

Forschungsberichte aus dem
wbk Institut für Produktionstechnik
Karlsruher Institut für Technologie (KIT)

Germán González Fernández

**Microstructure-Based Finite-Element
Prediction of Surface Integrity with
Bayesian-Informed Wear States**
Application to Longitudinal Turning of AISI 4140

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Doktors der Ingenieurwissenschaften (Dr.-Ing.)

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Editors' Foreword

The rapid and efficient implementation of innovative technologies will become the crucial economic factor for manufacturing companies in the context of economic globalization. Universities can significantly contribute to the competitiveness of the industry as value creation partners by developing scientific foundations as well as new methods and technologies, and by actively supporting the implementation process into practical applications.

Against this backdrop, this series aims to report on the latest research findings of the wbk Institute of Production Science at the Karlsruhe Institute of Technology (KIT). Our research focuses on enhancing the performance of additive and subtractive manufacturing processes, production equipment, and process automation, as well as on the comprehensive analysis and optimisation of production systems and networks. Both technological and organizational aspects are considered in these endeavors.

Prof. Dr.-Ing. Jürgen Fleischer

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Prof. Dr.-Ing. Frederik Zanger

Author's Preface

This dissertation was prepared at the wbk Institute of Production Science at the Karlsruhe Institute of Technology (KIT). The research was carried out within the Manufacturing and Materials Technology group and was motivated by the ongoing effort to advance the scientific understanding and technological control of surface integrity in machining processes. The work developed at the intersection of numerical modelling, experimental process analysis, and sensor development, and benefited greatly from the interdisciplinary research environment at the institute.

I would like to express my sincere gratitude to Prof. Dr.-Ing. habil. Volker Schulze for his excellent supervision, his guidance throughout the entire project, and the considerable freedom he afforded me in shaping the scientific direction of this work. My thanks also go to Prof. Dr.-Ing. Julius Schoop for kindly serving as second reviewer and for enabling a research stay at the Institute of Sustainable Manufacturing at the University of Kentucky, which broadened the methodological and conceptual perspective of the dissertation.

I gratefully acknowledge the Karlsruhe House of Young Scientists (KHYS) for its financial support of the international research stay. I would also like to thank my colleagues at the wbk for creating a stimulating and supportive research environment, for their technical assistance, and for the many valuable discussions that contributed to the development of this dissertation. My sincere appreciation also goes to the students who supported the experimental work, sensor fabrication, and data analysis through their theses and research activities.

Finally, I would like to thank my family and friends for their patience, encouragement and unwavering support throughout the doctoral process. Their confidence and continuous backing made the completion of this dissertation possible.

Karlsruhe, July 2026

Germán González Fernández

Abstract

This thesis develops a hybrid modelling and sensing framework for wear-dependent prediction of surface integrity in machining. The work is motivated by the need for mechanism-based, uncertainty-aware prediction of microstructural refinement in the machined surface under evolving tool wear conditions, a capability that remains insufficiently addressed by existing models and is rarely available for process-accompanying application. To address this gap, a microstructure-informed finite-element (FE) model of chip formation is first established and calibrated against dedicated orthogonal-cutting experiments using synchronised force, temperature and subsurface characterisation. The resulting thermo-mechanical fields serve as input to a post-processing step that evaluates microstructure-based metrics of near-surface grain refinement. The FE model is extended to 3D turning and executed across a factorial matrix of cutting parameters and tool-wear states to generate a high-fidelity database that underpins surrogate regression models for rapid, physics-consistent interpolation.

Complementing the simulation framework, thin-film thermistors and resistive wear tracks are integrated directly into industrial cutting inserts, enabling spatially resolved, high-bandwidth measurement of tool-tip temperature and flank wear under realistic operating conditions. These measurements support validation of the FE fields and provide sparse but informative data streams for wear estimation. Tool wear is modelled through an exponential degradation law embedded in a Bayesian inference formulation solved via Markov chain Monte Carlo. This approach yields posterior distributions for the wear parameters and wear trajectory, enabling early prediction with quantified uncertainty and principled transfer of information between cutting regimes.

The calibrated FE simulations, surrogate models and Bayesian wear inference are unified into an open-loop soft-sensor architecture for offline prediction and sequential updating of surface-integrity estimates when new wear observations become available. Posterior samples of wear are propagated through the surrogate layer to obtain predictive distributions of forces, temperatures and microstructural indicators such as ultrafine-grained surface layer thickness. This allows risk-aware assessment of surface quality and provides a decision-oriented interface for parameter selection and tool-change strategies. The framework transforms heterogeneous evidence from sensing, physics and data into uncertainty-aware predictions and establishes a basis for future on-machine, digital-twin and closed-loop applications.

Kurzfassung

Diese Dissertation entwickelt ein hybrides Modellierungs- und Sensorsystem zur verschleißabhängigen Vorhersage der Oberflächenintegrität in der Zerspanung. Ausgangspunkt ist der Bedarf an einer mechanismenbasierten, unsicherheitsbewussten Vorhersage der mikrostrukturellen Verfeinerung in der bearbeiteten Randzone unter sich entwickelnden Werkzeugverschleißzuständen, ein Aspekt, der von bestehenden Modellen nur unzureichend erfasst wird und für eine prozessbegleitende Anwendung bislang kaum verfügbar ist. Zur Schließung dieser Lücke wird zunächst ein mikrostrukturinformiertes Finite-Elemente-(FE)-Modell der Spanbildung aufgebaut und anhand gezielter orthogonaler Schnittversuche kalibriert, in denen Kräfte, Temperaturen und Gefügezustände erfasst wurden. Die resultierenden thermomechanischen Feldgrößen bilden die Grundlage eines Post-Processing-Schrittes zur Bewertung der oberflächennahen Kornfeinung. Das FE-Modell wird anschließend auf den 3D-Längsdrehprozess übertragen und über eine Matrix von Schnittparametern und Verschleißzuständen ausgeführt, wodurch eine hochaufgelöste Datenbasis entsteht, die regressionsbasierte Modelle für eine schnelle, physikkonsistente Interpolation ermöglicht.

Das Simulationskonzept wird durch Dünnschichtsensoren ergänzt, die direkt auf industrielle Wendeschneidplatten integriert wurden und hochfrequente Messungen von Schneidkanten-temperatur und Verschleiß unter realitätsnahen Einsatzbedingungen erlauben. Der Werkzeugverschleiß wird über ein exponentielles Degradationsgesetz beschrieben und in eine Bayessche Inferenzformulierung eingebettet, die mittels Markov Chain Monte Carlo gelöst wird. Dadurch entstehen Posteriorverteilungen der Verschleißparameter und der Verschleißtrajektorie, welche frühe Vorhersagen mit quantifizierter Unsicherheit sowie einen konsistenten Transfer von Information zwischen unterschiedlichen Schnittbedingungen ermöglichen.

Die kalibrierten FE-Simulationen, Surrogatmodelle und die Bayes'sche Verschleißinferenz werden schließlich in einer Open-Loop-Soft-Sensor-Architektur vereint, die Offline-Prognosen und eine sequentielle Aktualisierung der Oberflächenintegritätsschätzung bei Verfügbarkeit neuer Verschleißmessungen ermöglicht. Posterior-Samples des Verschleißes werden durch die Surrogatschicht propagiert, um prädiktive Verteilungen von Kräften, Temperaturen und mikrostrukturellen Kennwerten wie der nanokristallinen Randschichtdicke abzuleiten. Dies ermöglicht eine risikobewusste Bewertung der Oberflächenqualität und stellt eine entscheidungsorientierte Grundlage für die Auswahl von Prozessparametern sowie für Werkzeugwechselstrategien bereit. Das Gesamtsystem transformiert heterogene Daten zu operativ nutzbaren Vorhersagen und schafft damit eine Grundlage für digitale Zwillinge und zukünftige Closed-Loop-Regelstrategien in der spanenden Fertigung.

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Abbreviations and Symbols

Abbreviation	Description
3MA	Micromagnetic Multiparameter Microstructure and Stress Analysis
AE	Acoustic Emission
AI	Artificial Intelligence
ANN	Artificial Neural Network
BUE	Built-Up Edge
CCD	Charge-Coupled Device
CFD	Computational Fluid Dynamics
CNC	Computer Numerical Control
CVD	Chemical Vapor Deposition
DAQ	Data Acquisition
DIC	Digital Image Correlation
DLC	Diamond-Like Carbon
DSA	Direct/Downhill Simplex Algorithm (parameter optimisation)
DSS	<i>Dünnschichtsensorik</i> (Thin-Film Sensor Technology)
DRX	Dynamic recrystallisation
EDM	Electrical Discharge Machining
EPD	Electrophoretic Deposition
FEM (FE)	Finite Element Method (Finite Element)
FIB	Focused Ion Beam
IICC	Ion-Induced Channeling Contrast
IR	Infrared
JC	Johnson–Cook (constitutive model)
LSF	Least Squares Fitting
MCMC	Markov Chain Monte Carlo
MEMS	Micro-Electro-Mechanical Systems
MTL	Material Transfer Layer(s)
NUTS	No-U-Turn Sampler
PCB	Printed Circuit Board
PVD	Physical Vapor Deposition
RBF	Radial basis function
RMS	Root Mean Square
RTD	Resistance Temperature Detector
SEM	Scanning Electron Microscope
SI	Surface Integrity

SIMS	Secondary Ion Mass Spectrometry
SPD	Severe Plastic Deformation
UFG	Ultrafine Grained
VB	Flank wear land width
WC–Co	Tungsten Carbide–Cobalt

Symbol	Description	Unit	Context
a_p	Depth of cut	mm	Process
f	Feed per revolution	mm/rev	Process
v_c	Cutting speed	m/min	Process
h	Uncut chip thickness	μm	Process
h_c	Cut (deformed) chip thickness	μm	Process
$h_{\min}$	Minimum chip thickness	μm	Process
l_c	Cutting/contact length	mm	Process
r_β	Cutting edge radius	μm	Tool geometry
α	Clearance angle	$^\circ$	Tool geometry
γ	Rake angle	$^\circ$	Tool geometry
κ	Tool cutting edge angle	$^\circ$	Tool geometry
k	Thermal conductivity	$\text{W m}^{-1} \text{K}^{-1}$	Modelling
T	Absolute temperature	K	Modelling
T_0	Reference temperature	K	Modelling
T_m	Melting temperature	K	Modelling
$T_{\max}$	Peak surface temperature	$^\circ\text{C}$	Modelling
σ	Flow (true) stress	MPa	Modelling
σ_N	Normal stress	MPa	Modelling
τ_{fr}	Resulting frictional shear stress	MPa	Modelling
μ	Coulomb friction coefficient	—	Modelling
m	Shear friction factor	—	Modelling
$\dot{\varepsilon}, \dot{\varepsilon}_{pl}$	(Plastic) strain rate	s^{-1}	Modelling
$\varepsilon_{pl}, \bar{\varepsilon}_{pl}$	(Equivalent) plastic strain	—	Modelling
$\dot{\bar{\varepsilon}}_{pl}$	Equivalent plastic strain rate	s^{-1}	Modelling
φ	Shear angle	$^\circ$	Modelling
A, B, C	Johnson–Cook parameters	—	JC Modelling
n, m_{JC}	Johnson–Cook parameters	—	JC Modelling
$\dot{\varepsilon}_0$	Reference strain rate (JC)	s^{-1}	JC Modelling
Z	Zener–Hollomon parameter	—	DRX–Zener
Q	Activation energy for deformation	J/mol	DRX–Zener
R	Gas constant	$\text{J mol}^{-1} \text{K}^{-1}$	DRX–Zener
K_1, K_2	Grain-size law coefficients	—	DRX–Zener
$K_3, \dots, K_9$	DRX kinetic coefficients	—	DRX kinetics
$\varepsilon_{0.5}$	Strain at 50% recrystallisation	—	DRX kinetics
ε_{cr}	Critical strain for DRX onset	—	DRX kinetics

Symbol	Description	Unit	Context
X_{DRX}	Recrystallised volume fraction	–	DRX kinetics
ρ_c, ρ_w	Dislocation density in cell interiors / walls	m^{-2}	Dislocation model
ρ_{tot}	Total dislocation density	m^{-2}	Dislocation model
f_0, f_∞	Cell-wall volume fraction	–	Dislocation model
$\tilde{\gamma}_r$	Reference shear strain	–	Dislocation model
$\dot{\gamma}_r$	Equivalent shear rate	s^{-1}	Dislocation model
$\dot{\gamma}_0$	Reference shear rate	s^{-1}	Dislocation model
M_T	Taylor factor	–	Dislocation model
b	Burgers vector	m	Dislocation model
α^*, β^*, k_0	Dislocation model coefficients	–	Dislocation model
K_{dd}	Grain-size scaling	m^{-1}	Dislocation model
d, d_{t+1}	Grain size (current / updated)	μm	Dislocation model
d_0	Initial grain size	μm	Dislocation model
d_{DRX}	DRX grain size (steady/limit)	μm	Dislocation model
$\gamma_{\text{gb}}(T)$	Grain-boundary energy	J/m^2	Helmholtz-model
$\Omega(T)$	Stored-energy fraction	–	Helmholtz-model
ω_1, ω_2	Stored-energy coefficients	–	Helmholtz-model
$a_{\text{gb}}, b_{\text{gb}}$	GB-energy linear coefficients	$\text{J}/\text{m}^2,$ $\text{J}/(\text{m}^2\text{K})$	Helmholtz-model
β_{rx}	Recrystallisation efficiency	–	Helmholtz-model
T_{TF}	Temperature Thin-film sensor	$^\circ\text{C}$	Sensing
T_t, T_w	Thermocouple temperature	$^\circ\text{C}$	Sensing
$R(T)$	Sensor resistance at T	Ω	Sensing
R_0	Sensor resistance at T_0	Ω	Sensing
F_c	Cutting force	N	Process forces
F_f	Feed force	N	Process forces
F_p	Passive force	N	Process forces
$z_{\text{gs} < X}$	Thickness with $> 95\%$ grains $< X$	μm	Surface Integrity

1 Introduction

Machining has been refined over centuries and is grounded in physics-based descriptions of plastic deformation, frictional contact, heat generation, and microstructural evolution. Yet pronounced variability persists in industrial environments. Fluctuations in workpiece properties, tool condition and wear, lubrication, chip evacuation, and measurement noise introduce stochastic elements that complicate prediction and control. As a result, purely *a priori* process planning can deviate from targeted product characteristics, particularly for attributes governed by the near-surface material state.

Surface engineering addresses this challenge by explicitly linking process variables to the functional performance of the surface layer. Residual stresses, work hardening, microstructural refinement, and topography jointly determine fatigue strength, wear resistance, and corrosion behaviour. In turning and related processes, these attributes are acutely sensitive to the thermal–mechanical history in shear zones and to time-varying disturbances such as tool wear.

To achieve robust compliance with surface-integrity targets, control solutions must combine (i) physics-based understanding of chip formation and heat flow, (ii) process-integrated sensing to observe latent states, and (iii) data-driven inference to cope with uncertainty. Figure 1.1 summarises the control architecture developed in the DFG Priority Programme SPP 2086 “Surface Conditioning in Machining”.

In this framework, process parameters are adjusted in a feedback loop using *soft sensors* that fuse heterogeneous information sources—physical sensors, process models, and expert knowledge—into real-time estimates of otherwise unmeasurable quantities (González & Schulze 2024). This concept is essential when direct measurement is infeasible (e.g., subsurface microstructure during cutting) or when single sensors provide incomplete information.

The present work advances a hybrid soft-sensing approach for uncertainty-aware surface-integrity prediction and monitoring in longitudinal turning of AISI 4140. At a high level, the methodology integrates a microstructure-based finite-element model of chip formation (providing time-resolved fields of strain, strain rate, and temperature in the surface layer), tool-integrated thin-film sensors for high-resolution observation of tool-side temperature and progressive wear under production-relevant conditions, and Bayesian inference to estimate and forecast the wear state from sparse measurements with quantified uncertainty. The combination is deliberately modular: physics provides mechanistic structure, sensing constrains key latent states in situ, and probabilistic updating propagates uncertainty from data to decisions.

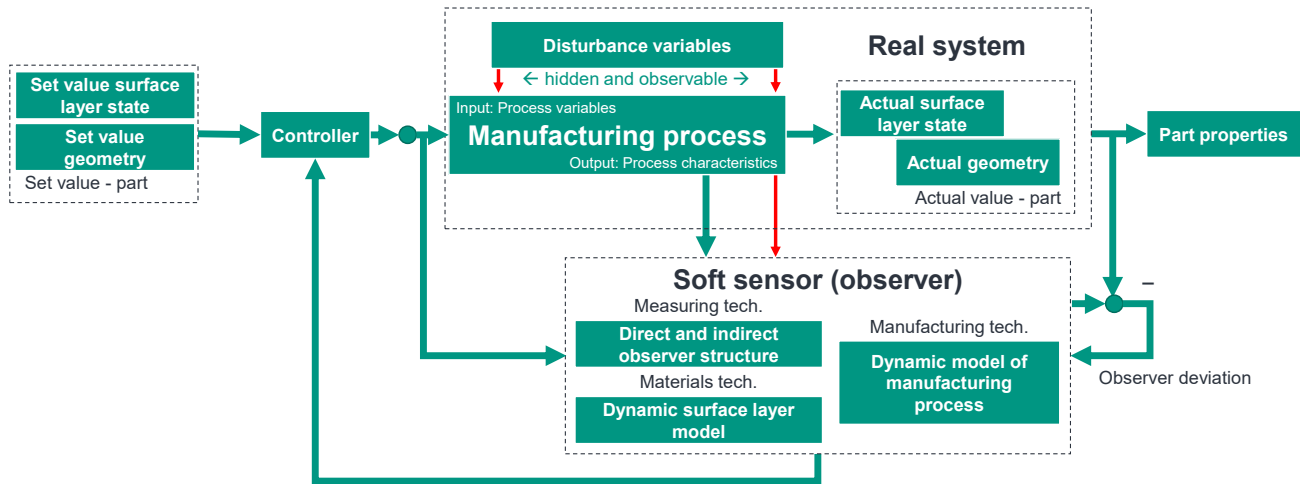


Figure 1.1: Process-control architecture for surface conditioning in machining within the DFG Priority Programme SPP 2086 (Stampfer & González et al. 2021a).

The structure of this dissertation is organised as follows. Chapter 2 provides a comprehensive review of the state of the art in surface integrity, process monitoring and hybrid modelling concepts, establishing the scientific context and identifying the methodological gaps addressed in this work. The precise research objectives, scope and validation strategy are formulated in Chapter 3. Chapter 4 introduces the experimental platforms and the fabrication of thin-film sensors, and details the constitutive modelling and microstructure-based formulation employed for post-processing of FE fields. Chapters 5 and 6 present the calibrated two- and three-dimensional thermomechanical cutting simulations and their experimental validation in terms of forces, tool-side temperatures and microstructural response. Chapter 7 develops the Bayesian framework for tool-wear inference and describes its integration with the FE-based surface-integrity predictions for early-stage forecasting and decision support. Finally, Chapter 8 synthesises the main scientific contributions, discusses the limitations and generalisability of the modelling chain, evaluates the implications for digital-twin concepts in machining, and outlines directions for future research.

2 Fundamentals and State of the Art

This chapter introduces the fundamentals of turning and the resulting surface characteristics of machined components. The concept of *surface integrity* is defined and its main drivers and metrology approaches are reviewed, with emphasis on the link between surface integrity and component performance. The foundations of thin-film, tool-integrated sensing for spatially resolved measurements are outlined. Finally, modelling approaches based on finite elements and Bayesian inference are introduced, as they are used throughout this work to simulate and predict the evolution of the surface state during machining.

2.1 The Turning Process

Turning (DIN 8589) removes material from a rotating workpiece by means of a cutting tool and is ubiquitous for manufacturing shafts, bearings, and gear components. Key process parameters are cutting speed v_c , feed rate f (feed per revolution), and depth of cut a_p . The effective cutting engagement is governed by tool and holder geometry via rake angle γ and clearance angle α . Tool macro-/microgeometry—such as chip-breaker features, nose radius r_e , and edge radius r_β —strongly affects chip formation and contact conditions. Figure 2.1 sketches the idealised orthogonal cutting configuration and a longitudinal turning setup, highlighting the principal kinematics and force components. Orthogonal cutting serves as a simplified process for analysing chip formation, forces, and wear, and for understanding how v_c , f , and tool geometry shape the thermo-mechanical fields.

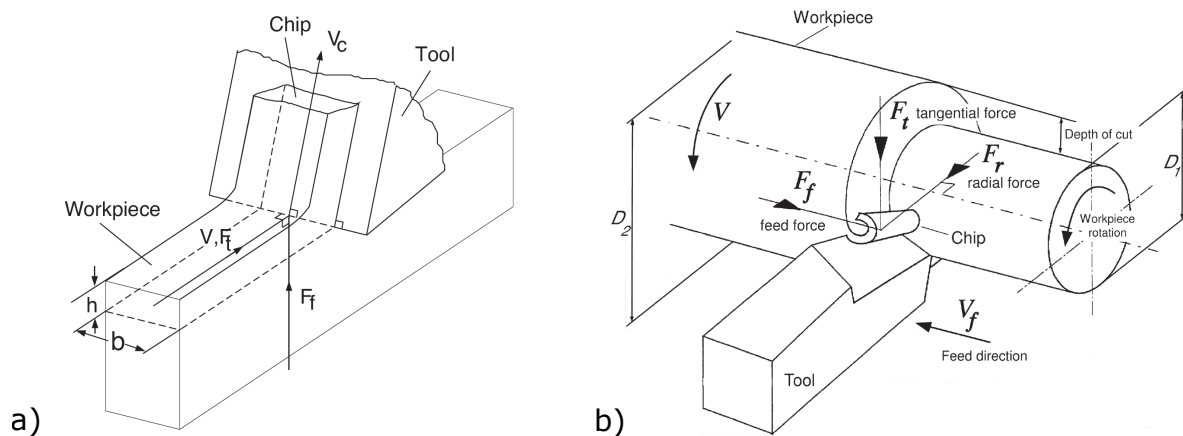


Figure 2.1: Process kinematics: a) Orthogonal cutting; b) Turning – Altintas (2012).

Machining of metallic materials generates severe plastic deformation (SPD) at high strain rates and elevated temperatures in the deformation zone ahead of the cutting edge. These conditions alter the microstructure of both the chip and the near-surface of the workpiece (Jawahir & Brinksmeier et al. 2011). Deformation and heat generation are classically partitioned into three regions: the primary shear zone (chip formation), the secondary zone at

the tool–chip interface, and the tertiary zone at the tool flank–workpiece interface (Childs 2010). Owing to coupled mechanical and thermal loads, the resulting thermo-mechanical processing can modify surface integrity to depths of 5 μm to 1000 μm , depending on material, tool geometry, cooling/lubrication, and process parameters (Liao & Monaca et al. 2021). Figure 2.2 summarises the orthogonal representation with the three zones, characteristic heat sources, and heat partitioning. Plastic work in the primary zone and frictional sliding in the secondary and tertiary zones are the dominant heat sources (Rech & Arrazola et al. 2013).

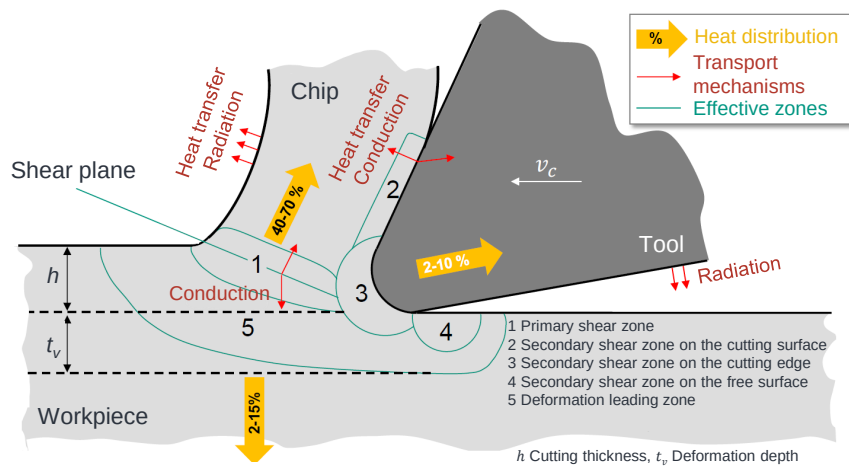


Figure 2.2: Orthogonal cutting representation with primary/secondary/tertiary zones, heat sources, and heat partition. Adapted from Warnecke (1974).

The machining tribosystem (tool–workpiece–environment) governs contact mechanics and thus chip formation. Figure 2.3 depicts the interacting mechanisms of adhesion, ploughing, and plastic deformation at the interfaces (Schumacher & Murrenhoff 2010). The system is highly dynamic: local sticking and sliding regions can coexist along the edge radius, ploughing beneath the flank face contributes to passive forces, and built-up edge (BUE) formation modifies geometry and friction in time.

The tool can experience nominal contact pressures up to ~ 3 GPa, sliding speeds approaching 10^3 m/min, and local temperatures exceeding 10^3 °C, leading to combined abrasion, adhesion, diffusion/oxidation wear, plastic blunting of the edge, thermal–mechanical fatigue, and brittle chipping (Klocke & König 2008).

These processes are rooted in frictional interactions. The (global) *apparent* coefficient of friction $\mu_{\text{app}} = F_f/F_N$ is often inferred from force measurements, but it does not reflect spatially varying *local* friction. Stick–slip behaviour is a prominent example: local stick regions (elastic storage, $\mu_{\text{loc}} > \mu_{\text{app}}$) alternate with sliding regions ($\mu_{\text{loc}} < \mu_{\text{app}}$), producing a lower apparent friction at the system level (Adams 1998).

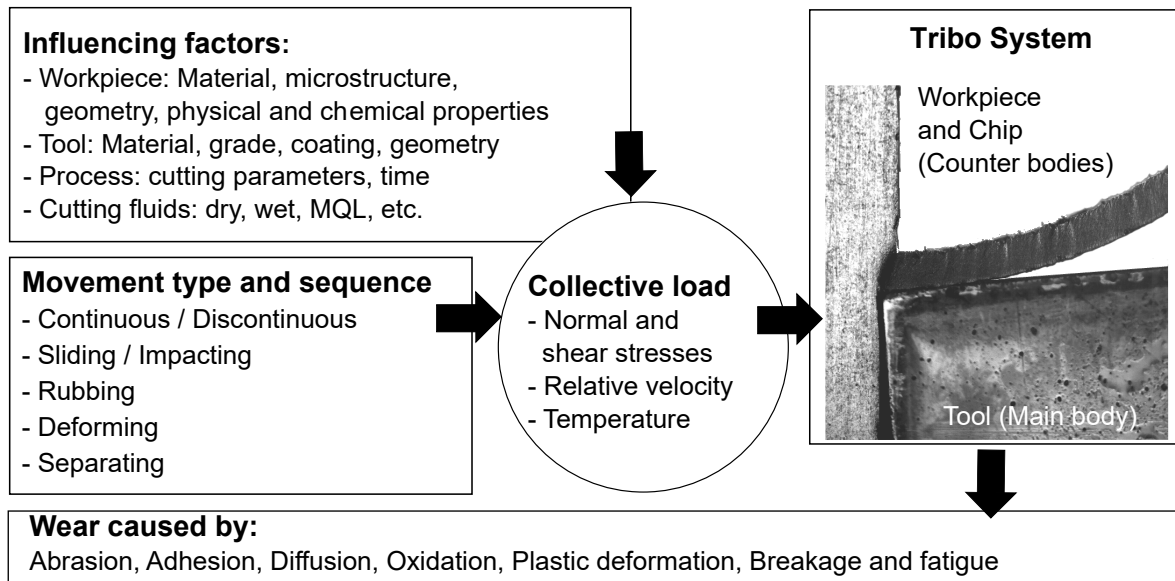


Figure 2.3: Machining tribosystem, adapted from Schumacher & Murrenhoff (2010).

Coulomb friction should thus be regarded as an empirical approximation valid mainly for dry, elastic contact. Contact transitions (stick–slip), BUE formation, and wear-induced geometry changes modulate local friction and heat generation. In practice, a combined Coulomb–shear law with temperature/pressure dependence offers a tractable approximation, but its parameters are uncertain.

The mathematical models describing friction are summarised as follows:

Coulomb Friction	Shear Friction (Tresca)	Combined Friction
$\tau_{fr} = \mu \cdot \sigma_N$	$\tau_{fr} = m \cdot \frac{\sigma_{fs}}{\sqrt{3}}$	$\tau_{fr} = \min \left(\mu \cdot \sigma_N, m \cdot \frac{\sigma_{fs}}{\sqrt{3}} \right)$

Progressive tool wear deteriorates the contact conditions, raising frictional work and heat generation. The ensuing increase in mechanothermal load intensifies adhesion and abrasion and promotes material transfer. These changes affect process stability and alter surface integrity through work hardening, residual-stress development, microstructural transformation and increased roughness. Their influence on fatigue and tribological performance depends on the type, magnitude and spatial distribution of the resulting surface modification.

2.2 Surface Integrity in Machining Operations

The concept of surface integrity encompasses the process-induced properties, including topographic, metallurgical, and micromechanical characteristics, which are influenced by machining processes and extend from the workpiece surface into the subsurface volume. It is defined as the inherent or enhanced condition of a surface resulting from machining or other

surface generation operations (Kahles & Field 1967), playing a critical role in determining component performance. Surface integrity is shaped by the interactions of mechanical, thermal, and chemical forces during machining, which cause physical and chemical changes to the workpiece material (Jawahir & Brinksmeier et al. 2011). Key characteristics of surface integrity include surface topography (e.g., roughness parameters), material microstructure (e.g., phase, grain size, dislocation density), surface and subsurface hardness, and residual stresses. Surface topography affects the quality and functional performance of the machined surface, while the microstructure significantly influences material properties such as fatigue strength and wear resistance. Residual stresses, resulting from thermo-mechanical loading, are critical for dimensional stability and mechanical performance. Collectively, these factors are crucial for optimising machining processes, as they directly impact the functional performance and durability of machined components.

La Monaca et al. categorise the mechanisms generating surface integrity into four main groups based on the dominant type of loading or interaction during the machining process: mechanical dominant, thermal dominant, chemical dominant, and combined loading. These classifications help in understanding how different manufacturing processes and their conditions affect the final properties of a machined surface (Liao & Monaca et al. 2021) and (Monaca & Murray et al. 2021).

- **Mechanically Dominated:** Changes in surface integrity are primarily caused by mechanical forces, resulting in deformation, strain, and residual stresses. Typical effects include variations in surface roughness, micro-crack formation, plastic deformation, work hardening, and phase transformations due to severe plastic deformation.
- **Thermally Dominated:** Heat generation during machining significantly impacts surface and subsurface properties. Thermal effects induce microstructural changes (e.g., recrystallisation, grain growth), alterations in residual stresses, oxidation, and thermal damage such as surface burns, which are characteristic of grinding processes.
- **Chemically Dominated:** Surface integrity changes result from chemical reactions between the workpiece material and the environment or cutting fluids. These effects include modifications to surface chemistry, corrosion resistance, new phase formation, and diffusion-driven microstructural changes.
- **Combined Loading:** Many machining processes involve simultaneous mechanical, thermal, and chemical influences, leading to complex surface integrity alterations. Combined loading results in changes to microstructure, surface chemistry, residual stresses, and surface topography.

Figure 2.4 provides a comprehensive illustration of the multi-faceted concept of surface integrity in machined components. In Figure 2.4a, a detailed schematic of a machined surface, originally proposed by (Scholtes 1991), highlights the critical elements that define surface integrity. These elements include surface texture, microstructural hardness (HV), subsurface cracks, and the distribution of residual stresses—perpendicular ($\sigma_{\perp}$) and parallel ($\sigma_{\parallel}$) to the machined surface (Scholtes 1991). Building on the classification of (Liao & Monaca et al. 2021), Karpuschewski et al. proposed the “Triangle of Process Loads” shown in Fig. 2.4b. At each vertex of the triangle lies a domain where one type of loading predominates, while the edges represent transitional zones where overlapping effects from multiple load types occur (Karpuschewski & Kinner-Becker et al. 2022).

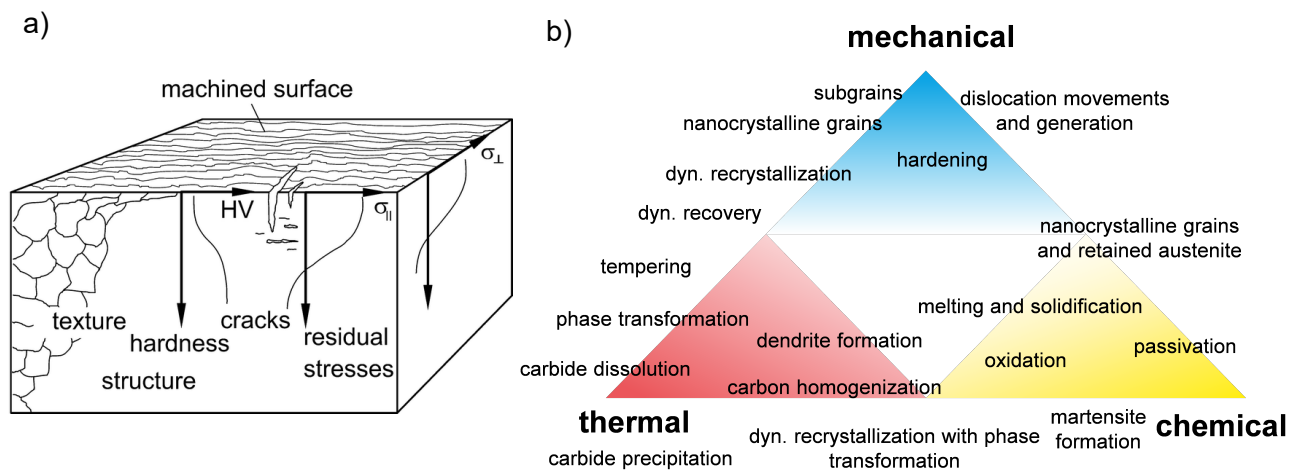


Figure 2.4: a) Surface Integrity characterisation (Scholtes 1991); b) Triangle of Process Loads and load dominance (Karpuschewski & Kinner-Becker et al. 2022).

The microstructural surface layer of metals is subject to diverse physical mechanisms during machining, affected by factors such as alloying constituents, temperature profiles and peak temperatures. These variables significantly influence the phase fractions in metals. For instance, high machining temperatures can lead to the formation of austenite in pearlitic-ferritic steels, which, upon rapid cooling, may transform into martensitic structures or intermediate microstructures. These transformations often result in a hardened, untempered surface layer with increased brittleness and a propensity for crack growth (Kahles & Field 1967). Parametric control over cutting speed, feed rate, depth of cut, and coolant application is vital in tailoring the surface layer state. Furthermore, the geometry of the cutting tool, especially the cutting edge radius, has been shown to influence surface recrystallisation (Schulze & Zanger et al. 2013) and the magnitude of compressive residual stresses (Denkena & Leon et al. 2010). The ratio of the cutting edge radius to chip thickness directly correlates with the degree of surface layer recrystallisation, impacting the material's mechanical properties (Ambrosy & Zanger et al. 2015). As the uncut chip thickness becomes small relative to the cutting-edge

radius, the ploughing zone expands, producing more deeply affected subsurface regions and larger force components normal to the workpiece surface (Segebade & Zanger et al. 2016).

The severe plastic deformation caused by machining can result in the formation of small-angle grain boundaries, subgrains, and dynamic recrystallisation at high dislocation densities (Huang & Hansen et al. 2003). Tool wear exacerbates the thermal load on the workpiece by expanding the contact and friction areas, subsequently affecting phase transitions and hardness (Komanduri & Hou 2001). The density of dislocations, indicative of plastic deformation, is known to increase during machining, leading to work hardening. Elevated stresses, strains, and temperatures promote the formation of large-angle grain boundaries and new grains (Totten & Howes et al. 2004). According to the Hall–Petch relationship, grain refinement generally increases strength and hardness; its influence on brittleness and crack propagation additionally depends on phase composition, residual stress and the deformation history (Hall 1951; Petch 1953).

Nanocrystalline edge layers, often referred to as "white layers" due to their appearance post-etching, scatter light and are unresolved under an optical microscope. These layers possess a hard and brittle nature that can initiate and propagate cracks, impacting the fatigue strength of the finished product (Shaw 1996). Two forms are commonly distinguished: the mechanically induced white layer (M-WL) and the thermally induced white layer (T-WL), both of which may contain grains in the nanometre range. The M-WL arises from severe plastic deformation at temperatures low enough to avoid phase transformations, while the T-WL involves grain refinement coupled with phase transformations due to thermal loads (Liao & Monaca et al. 2021).

The optimisation of surface properties represents a key lever for enhancing component performance. While the formation of severely plastically deformed near-surface layers is often detrimental to fatigue life owing to strain localisation, embrittlement, and an increased crack-initiation tendency, beneficial effects can arise when microstructural modification is dominated by mechanically induced grain refinement and compressive residual stresses rather than thermally driven damage. Under such mechanically dominated conditions, intensive machining or surface finishing processes can promote ultrafine grain structures and high dislocation densities, thereby improving strength, hardness, and wear resistance, even in high-strength materials.

Gerstenmeyer et al. demonstrated this potential for hardened AISI 4140 shafts: compared with conventional turning, a complementary machining strategy employing a burnishing effect from the primary flank face under reverse feed motion resulted in predominantly mechanically induced surface conditioning. This translated into a substantial enhancement of fatigue

resistance, with the fatigue limit increased by approximately 35% at a 95% probability of failure (Gerstenmeyer & Zanger et al. 2018).

2.2.1 Surface Integrity Assessment Methods

Surface integrity analysis is essential for linking machining processes to the functional performance of components. It involves assessing surface and subsurface states — such as roughness, hardness, residual stress, and microstructure — whose evolution governs fatigue, wear, and corrosion resistance. Methods differ in invasiveness, measurement scale, and suitability for in- or off-process use, requiring careful selection depending on application context.

Tactile methods such as stylus profilometry deliver precise and reliable roughness measurements but are inherently slow and invasive, limiting their use to off-process inspections in controlled environments (Jenkins & Mansfield 2013). Optical techniques, including confocal microscopy, white-light interferometry, and laser scanning, provide rapid, non-contact evaluation of surface texture and topography. While accurate and non-invasive, their sensitivity to vibrations and contamination typically confines them to laboratory or post-process applications.

For microstructural evaluation, high-resolution electron-based methods such as SEM, TEM, and EBSD offer detailed insights into grain orientation, phase distribution, and deformation structures (Schwarzer 2009). These methods, however, require destructive sample preparation and are therefore restricted to off-process characterisation. Complementarily, X-ray diffraction (XRD) enables non-destructive quantification of residual stresses, strain hardening, and phase transformations, making it one of the most widely applied techniques for off-process structural assessment (Noyan & Cohen 1987). Micro- and nanomechanical properties such as hardness and elastic modulus can be probed using nanoindentation. Although locally invasive, this technique provides quantitative information on the effects of machining-induced microstructural changes, coatings, or thermal exposure.

In-process and non-invasive approaches are particularly valuable for real-time monitoring and early defect detection. Acoustic emission (AE) captures stress waves generated during plastic deformation, crack initiation, or chip formation, enabling dynamic assessment of surface damage during machining. Micromagnetic methods, including Barkhausen noise, incremental permeability, and multi-frequency eddy current analysis, allow in-situ evaluation of residual stresses, hardness, and phase variations in ferromagnetic materials (Güray & Böttger et al. 2023). Barkhausen noise analysis is especially effective for detecting grinding burns and phase transformations, making it well suited for quality assurance in hardened surfaces. Recent studies have shown the successful integration of AE and micromagnetic sensors into

machining centres, demonstrating their potential for robust process monitoring (Böttger & González et al. 2024; Diaz Ocampo & Aubart et al. 2024).

No single technique provides a complete characterization of surface integrity. Instead, complementary use of topographic, structural, and micromechanical methods is required to capture the multi-scale and multi-physics nature of process–surface interactions. Table 2.1 summarizes the discussed techniques according to process integration, invasiveness, and application domain.

Table 2.1: Classification of Surface Integrity Assessment Methods

Method	In/Off Process	Invasive	Key Application
Stylus Profilometry	Off	Yes	Roughness and profile measurement
Optical Techniques	Off	No	Surface texture and topography
SEM / TEM / EBSD	Off	Yes	Microstructure and grain orientation
XRD	Off	No	Residual stress and phase analysis
Nanoindentation	Off	Yes	Hardness and modulus assessment
Acoustic Emission (AE)	In	No	Crack initiation and dynamic damage monitoring
Micromagnetic Testing	In/Off	No	Residual stress, hardness, phase variations
Barkhausen Noise Analysis	In/Off	No	Grinding burn detection and stress evaluation
Eddy Current Testing	In/Off	No	Crack and defect detection in conductive materials
Laser Ultrasonics	In	No	Residual stress, thickness, and defect analysis
Thermography	In	No	Surface temperature mapping and defect visualisation

2.3 Thin-Film Sensors for Spatially Resolved Measurement

An alternative class of surface integrity assessment methods relies on empirical correlations between measurable process response variables and the resulting surface condition. Although typically less reliable than direct physical sensing techniques, these approaches provide cost-effective monitoring by exploiting data already available from machine tool sensors or logic controllers, such as spindle power consumption or vibration signals. While long established in tool condition monitoring and predictive maintenance, such indirect indicators have also demonstrated potential for inferring surface integrity.

Recent research has focused on integrating thin-film sensor technology directly into cutting tools, offering unique opportunities for in-situ and spatially resolved monitoring in the tool–workpiece contact zone. Such resolution is unattainable with conventional measurement technologies. Micro-Electro-Mechanical Systems (MEMS) processes enable the fabrication

of thin-film thermocouples and resistive sensors through deposition (PVD, CVD), lithography, and etching, with sensing elements defined at the micrometer scale. Although no commercial cutting tools currently employ this technology, academic prototypes have demonstrated its potential to capture process temperatures and tool wear with unprecedented precision, thereby enhancing understanding and modelling of machining processes.

2.3.1 In-tool Integrated Temperature Sensors

Compared to conventional embedded thermocouples, thin-film sensors offer a decisive advantage by enabling placement much closer to the cutting edge. This proximity allows for spatially resolved temperature measurements with far greater accuracy. While the positioning accuracy of embedded thermocouples is typically in the millimetre range—limited by wire diameters of 0.5 mm or larger—thin-film sensors achieve micrometre-level precision, with sensing elements as narrow as a few tens of microns.

These miniaturised thermocouples are typically fabricated by layering dissimilar metals such as Ni–NiCr or NiCr–NiSi on rake or flank faces of carbide inserts. Hot junctions are formed where these materials intersect, enabling high-resolution temperature tracking. Early work by Sugita et al. (Sugita & Ishii et al. 2015) demonstrated the feasibility of this concept using micro-grooved thermocouples deposited on cemented tungsten carbide tools. Subsequent research by Basti et al. (Basti & Obikawa et al. 2007) further highlighted the advantages of thin-film sensors in orthogonal machining of aluminum alloys.

The thin-film system is constructed by stacking multiple functional layers that provide insulation, wear protection, and the sensory capability itself. Thermoelectric thin-film sensors (Figure 2.5a) exploit the Seebeck effect, where a voltage arises due to a temperature gradient between dissimilar conductors. The voltage magnitude depends on the difference in Seebeck coefficients and is proportional to the temperature difference (Seebeck 1822).

An alternative approach is resistive thin-film sensing (Figure 2.5b), which relies on the temperature dependence of electrical resistance. Resistance thermometers are categorised into Positive Temperature Coefficient (PTC) and Negative Temperature Coefficient (NTC) types. While more sensitive to material properties and geometry than thermocouples, resistive thin-film sensors provide several advantages: lower production cost, greater flexibility in design, and higher potential for miniaturization. These properties enable dense layouts for high spatial resolution.

Several studies highlight their potential for precision monitoring. Yoshioka et al. (Yoshioka & Hashizume et al. 2004) integrated a platinum resistance microsensor onto the rake face of a diamond tool for turning Al–Mg alloys, achieving rapid response with minimal thermal lag.

Hayashi et al. (Hayashi & Yoshioka et al. 2008) refined this design with a meander-shaped sensing element and integrated bridge electronics, demonstrating improved stability and signal quality. More recently, Plogmeyer et al. (Plogmeyer & González et al. 2020) developed a Cr-based resistive sensor protected by Al_2O_3 for turning AISI 4140, explicitly addressing the influence of machining forces on measurement accuracy.

Despite their promise, thin-film temperature sensors face challenges in calibration and durability. Conventional calibration methods—such as oil baths, heat plates, or infrared cameras—have been applied (Biermann & Kirschner et al. 2013). Protection against wear remains a major concern, with Al_2O_3 or similar oxides commonly used as protective and insulating layers (Bobzin & Brögelmann et al. 2020). Compared to conventional thermocouples, thin-film sensors produce smaller voltage signals, making accurate signal acquisition and calibration critical. Nevertheless, the combination of MEMS precision, high spatial resolution, and potential for in-situ application makes thermoresistive thin-film sensors particularly attractive for surface integrity monitoring.

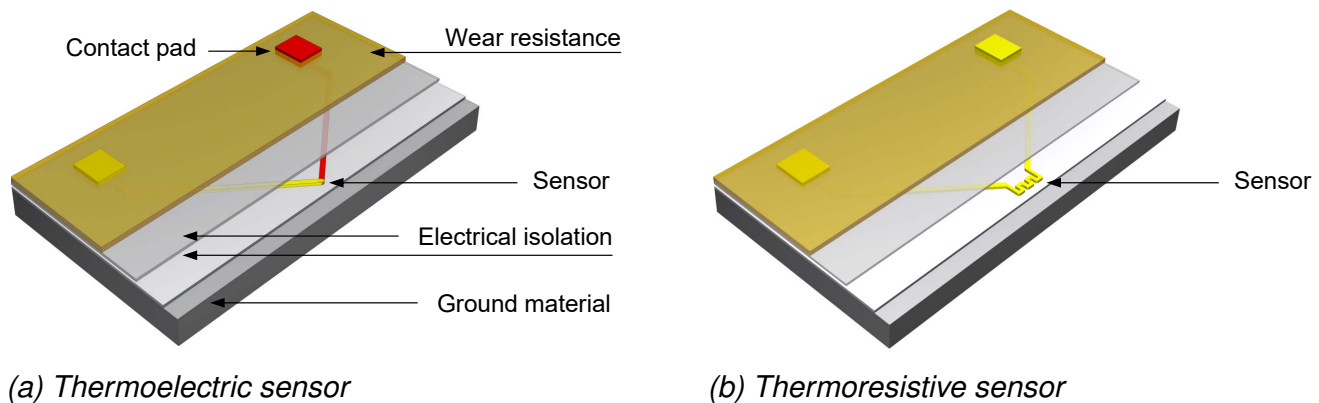


Figure 2.5: Classification of thin-film sensor technologies according to the measuring principle (González & Plogmeyer et al. 2023).

2.3.2 In-tool Integrated Wear Sensors

Beyond temperature measurement, thin-film sensors also enable in-situ monitoring of tool wear. One common strategy employs multiple conductive tracks patterned into rake or flank faces. As wear progresses, these tracks are successively broken, resulting in measurable resistance changes that directly indicate wear evolution (Schmaljohann & Hagedorn et al. 2015). Alternative approaches use ferromagnetic coatings whose magnetic response changes as the layer is worn, providing an additional sensing modality (Lüthje & Bandorf et al. 2004). More recent designs have refined resistive concepts by arranging multiple conductive paths in parallel, enabling predictable resistance changes with wear severity. This approach allows

real-time estimation of flank wear land width or crater depth using only two external contacts, as demonstrated by Plogmeyer et al. (Plogmeyer & González et al. 2021).

In summary, thin-film sensor technology offers a pathway toward spatially resolved, in-situ measurement of process variables highly relevant to surface integrity. Temperature and wear monitoring at micrometer resolution near the cutting edge provides unique insights into the thermo-mechanical loads acting on the workpiece surface and subsurface. These capabilities not only advance the modelling of machining processes but also support the development of tailored monitoring strategies for surface integrity. The following chapters describe the design, fabrication, and application of thin-film resistive temperature and wear sensors as developed in this work.

2.4 Modelling Machining Operations with Finite Element Analysis

Simulation is a key tool for the numerical analysis and optimisation of machining. It enables prediction of chip formation, tool–workpiece interaction, surface integrity, machine dynamics, and component distortion. Depending on the target variables, models—analytical or numerical—are structured across hierarchical levels (Table 2.2), each requiring tailored assumptions, inputs, and validation data.

Table 2.2: Levels of analysis in machining simulation (Segebade 2021)

Level	Objectives
Machine Dynamics	Stiffness, vibrations, path planning, geometric deviations
Process Kinematics	Local cutting parameters, kinematic roughness, path optimisation, cutting forces, tool deflection
Chip Formation	Time-resolved stress, strain, temperature fields; surface-layer states and chip flow

Chip-formation modelling begins with mesh generation, where tool and workpiece geometries are discretised (e.g., tetrahedra or hexahedra). Predictive accuracy depends strongly on mesh quality and local refinement in contact and shear zones. A reliable constitutive model is essential to capture the material response under coupled thermo–mechanical loading (stress, strain, strain rate, temperature, pressure). Accurate boundary conditions: Cutting speed, feed, edge geometry, friction/heat transfer, and coolant, are required to replicate realistic conditions. Tool–workpiece interaction is tracked via contact mechanics and frictional behaviour; these govern plastic deformation, chip morphology, heat generation, and ultimately the surface layer. Two-dimensional (2D) finite element simulations (Figure 2.6a) are widely used for

orthogonal cutting due to their computational efficiency and straightforward validation against experiments. Although geometric simplifications exclude three-dimensional effects, 2D models reliably capture core mechanisms such as chip formation, stress distribution, cutting forces, and first-order temperature fields in the primary and secondary zones, offering valuable insights into tool wear and thermal impacts on material properties. However, many industrially relevant processes involve oblique cutting, complex tool geometries, and heterogeneous boundary conditions that cannot be represented in 2D. In such cases, three-dimensional (3D) FEM simulations are indispensable. By resolving the full tool–workpiece engagement, 3D models capture effects such as chip flow in the third dimension, tool corner radius influence, and spatial variations in contact length, residual stress, and surface integrity. They also allow for the study of multi-tooth tools, interrupted cutting, and process kinematics representative of turning, milling, or drilling. The trade-off is a significant increase in computational cost and the need for advanced meshing and remeshing strategies to maintain accuracy during large deformations.

Beyond chip mechanics, FE simulations increasingly target *surface integrity* prediction, primarily in academic research. This requires constitutive/structural models that couple the thermo–mechanical fields to microstructural evolution: dynamic recrystallisation (DRX), grain refinement/growth, dislocation-density evolution, and phase transformations under high strain, strain rate, and temperature. Such models are generally empirical or semi-physical and are calibrated through metallography under controlled conditions.

Figure 2.6b illustrates a predicted grain-size distribution based on a DRX law dependent on strain and strain rate, enabling estimates of UFG/DRX layer depth and thickness. Limitations remain: 2D kinematics, empirical parameters, and the difficulty of reproducing extreme machining load paths with conventional material tests (especially strain rate). Recent work with orthogonal-cutting rigs and high-speed imaging (Schoop 2021) and with explicit coolant/lubrication effects (Bergmann & Denkena et al. 2023) aims to calibrate or derive models that better represent in-situ behaviour.

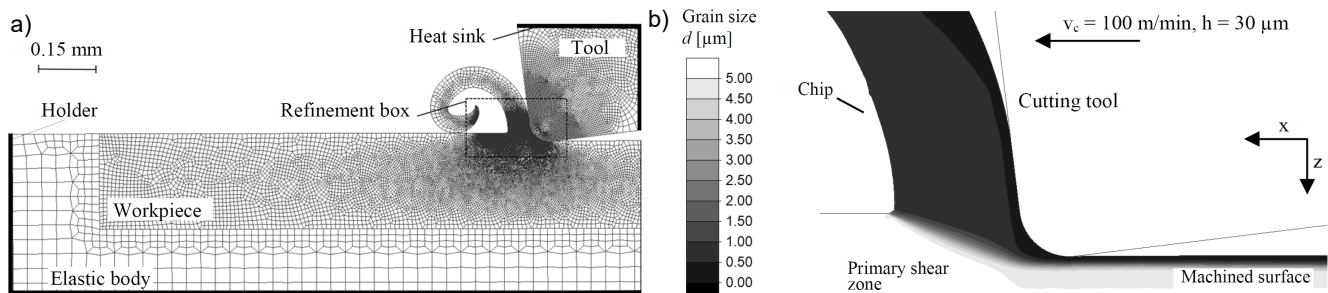


Figure 2.6: Chip formation FE simulation setup: a) 2D model of orthogonal cutting; b) Simulated workpiece grain size evolution (González & Segebade et al. 2019).

2.4.1 Material modelling: Stress–strain curve

Material modelling for chip-formation FE requires yield/flow behaviour and microstructural softening/hardening mechanisms (e.g., DRX, phase transformation), along with elastic modulus, heat capacity, and conductivity. Models range from phenomenological to physically based. The Johnson–Cook (JC) law is widely used for steels due to its compact form and robust calibration across strain rate and temperature (Johnson & Cook 1983). Using von Mises plasticity, the flow stress is

$$\sigma_f = (A + B \cdot \bar{\varepsilon}_{pl}^n) \cdot [1 + C \cdot \ln(\frac{\dot{\bar{\varepsilon}}_{pl}}{\dot{\varepsilon}_0})] \cdot \left(1 - \left(\frac{T - T_r}{T_m - T_r}\right)^m\right) \quad 2.1$$

where the first term applies a basic power law to describe the elasto-plastic behaviour, anchored in the yield strength A and modulated by hardening parameters B and n , contingent on the escalation of plastic strain $\bar{\varepsilon}_{pl}$. The model's second segment captures viscoplastic behaviour through the modulation of plastic strain rates $\dot{\bar{\varepsilon}}_{pl}$, using a reference strain rate $\dot{\varepsilon}_0$ and a constant C . The concluding term addresses thermal softening for temperatures exceeding T_r , dependent on the reference temperature T_r , the melting point T_m , and the modifier m_{JC} .

Phenomenological models are relatively easy to calibrate but limited in transferability; physically based models require broader datasets and internal variables, yet may generalise better (Melkote & Grzesik et al. 2017). A generic physically motivated form can be written as

$$\sigma_{fs,mp} = \sigma(\rho_1, \rho_2; \dot{\bar{\varepsilon}}_{pl}, T) \quad 2.2$$

where ρ_i denote internal state variables (e.g., dislocation densities, DRX fraction). To describe hardening due to plastic deformation, Tomé et al. (Tomé & Canova et al. 1984) and Voce (Voce 1948) proposed a constitutive relation that combines linear hardening with an exponential saturation term:

$$\sigma_y = (A + \sigma_1 + \theta_1 \cdot \bar{\varepsilon}_{pl}) \left[1 - \exp\left(-\frac{\theta_1 \cdot \bar{\varepsilon}_{pl}}{\theta_0}\right)\right]. \quad 2.3$$

Here, A denotes the initial yield stress, while σ_1 accounts for additional, strain-independent contributions to the flow stress. The parameter θ_1 acts as a hardening coefficient, scaling linearly with the accumulated plastic strain $\bar{\varepsilon}_{pl}$. The exponential term introduces a saturation behaviour, reflecting the tendency of metals to approach a limiting stress with increasing

plastic strain. The characteristic parameter θ_0 controls the rate at which this saturation occurs. The overline notation in $\overline{\varepsilon}_{pl}$ indicates an averaged or representative plastic strain, consistent with its use in continuum and FEM-based formulations, rather than an instantaneous local value. This formulation is therefore well suited to machining simulations, where the material experiences large strains and strain rates, but the hardening capacity is finite and governed by microstructural mechanisms such as dynamic recovery and recrystallisation.

2.4.2 Grain refinement

Grain refinement in machining is primarily driven by DRX once a critical strain or dislocation-density threshold is exceeded. New, equiaxed grains nucleate and grow, altering the near-surface microstructure. The extent depends on stress, temperature, and strain rate, governed by local thermo–mechanical energy input.

In FE chip simulations, DRX is commonly modelled via the Zener–Hollomon parameter, Z , which condenses strain-rate/temperature effects into a single kinetic driver; incremental forms tailored to machining were presented by Yanagimoto et al. (Yanagimoto & Karhausen et al. 1998). Ambrosy et al. used a Z -based model for AISI 4140 that also accounts for edge radius and uncut chip thickness, underscoring geometric sensitivity (Ambrosy & Zanger et al. 2015). Alternative approaches include thermodynamic irreversibility with critical-temperature activation (Buchkremer & Klocke et al. 2016) and dislocation-density based evolution (Estrin & Tóth et al. 1998; Estrin & Kim 2007), which have been applied to cutting of titanium alloys to predict surface refinement (Ding & Guo 2001).

The FE solution provides time-resolved thermo–mechanical paths $\{\overline{\varepsilon}(t), \dot{\overline{\varepsilon}}(t), T(t)\}$ in the surface layer. These histories are mapped to DRX drivers, for instance via the Zener–Hollomon parameter Z or through dislocation-density evolution laws, which represent the competing processes of dislocation storage and annihilation. From these formulations, the recrystallised fraction $X_{\text{DRX}}(t)$ and the ultrafine-grained layer thickness z_{UFG} can be predicted. Calibration of z_{UFG} and X_{DRX} against metallographic observations provides physics-informed constraints on the same FE boundary conditions that determine forces and tool/workpiece temperatures, thereby enabling multi-objective validation of the model.

2.4.3 Friction model

Interfacial friction on rake and flank governs heat generation, chip flow, contact pressures, wear, and thus surface integrity. The contact zone operates under extreme pressures, high strain rates, and steep thermal gradients; friction is spatially heterogeneous and time dependent. Following Zorev (Zorev 1963), the rake-face contact is partitioned into a *sticking* region near the cutting edge and a downstream *sliding* region. In turning, a similar transition exists across

the edge radius and onto the flank (tertiary contact), with additional ploughing under the flank.

Pure Coulomb friction ($\tau = \mu \sigma_n$) remains popular for robustness, but shear stress is bounded by the material shear flow stress. A combined Coulomb–shear law captures both regimes:

$$\tau_{\text{fr}} = \min(\mu \sigma_n, m k), \quad k = \frac{\sigma_{\text{fs}}}{\sqrt{3}}, \quad m \in [0, 1], \quad 2.4$$

with σ_n the contact pressure, μ the apparent friction coefficient, k the Tresca shear yield stress, and m a shear-friction factor. This reproduces sticking ($\tau \approx mk$) near the edge and sliding ($\tau \approx \mu \sigma_n$) further up the rake. Experiments and simulations indicate μ and/or m depend on local pressure, sliding speed, and especially temperature (Usui & Shirakashi 1982; Arrazola & Özel 2010). Accordingly, $\mu(p, v, T)$ or $m(p, v, T)$ and pressure-/temperature-dependent thermal contact conductance are often adopted. When in-situ tool-side temperature data are available (e.g., thin-film sensors), inverse identification of $\mu(\cdot)$, $m(\cdot)$, and conductance significantly reduces model bias.

2.4.4 Tool wear model

Wear kinetics are commonly represented by the Usui law (Usui & Shirakashi 1982), which relates local wear rate to contact pressure, sliding speed, and temperature via an Arrhenius term:

$$\dot{W} = A \sigma_n v \exp\left(-\frac{B}{T}\right), \quad 2.5$$

where $\dot{W}$ is the local wear-rate, σ_n the contact pressure, v the sliding speed, and T the interfacial temperature (K). The empirical constants A (scale) and B (activation) are fitted and typically differ for crater (rake) and flank wear. In FE, Eq. 2.5 is integrated along the contact to obtain wear depth; the evolved wear field is then mapped to geometry updates (explicit removal or morphing), with contact and thermal conditions recomputed on the updated surface. Arbitrary Lagrangian–Eulerian (ALE) or periodic remeshing strategies maintain mesh quality.

For abrasion-dominated regimes, Archard-type relations are used alone or combined with Usui:

$$\dot{h} = k_A \frac{\sigma_n}{H(T)} v, \quad 2.6$$

with $\dot{h}$ the local wear-depth rate, H the temperature-dependent hardness of the wearing partner, and k_A a wear coefficient. Diffusion/oxidation-assisted crater wear on coated tools can be represented by distinct (A, B) per layer/interface, with temperature-dependent transitions

to reflect coating softening or delamination. Validated cases include 2D wear progression on rake/flank (Yen & Söhner et al. 2002), coated tools and complex geometries (Binder & Klocke et al. 2015; Özel & Sima et al. 2010), and efficient 3D strategies that decompose wear into parallel 2D sections while retaining long-cut accuracy (Courbon & Fabre et al. 2021). Across models, two aspects are critical: (i) consistency between evolving wear geometry and contact/thermal boundary conditions (contact length, pressure footprint, heat partition), and (ii) calibration against data beyond forces (e.g., tool-side temperature and spatial wear metrics), since σ_n and T drive $\dot{W}$ exponentially in Eq. 2.5.

2.5 Bayesian Statistics in Machining

Machining processes are inherently stochastic: tool wear progresses non-uniformly, cutting forces fluctuate due to heterogeneous microstructures and chip segmentation, temperatures vary under transient contact, and all signals are corrupted by sensor noise. These uncertainties propagate to variability in surface integrity and tool life, limiting the reliability of purely deterministic models.

Bayesian inference offers a principled framework to represent and update uncertainty in such contexts. Unknown model parameters θ (e.g., wear-rate constants, friction coefficients, thermal conductivities) are treated as random variables, and prior knowledge $p(\theta)$ is combined with experimental data through the likelihood $p(y | \theta)$ to yield the posterior

$$p(\theta | y) = \frac{p(y | \theta) p(\theta)}{\int_{\Theta} p(y | \tilde{\theta}) p(\tilde{\theta}) d\tilde{\theta}}, \quad 2.7$$

where the denominator is the (typically intractable) model evidence. For datasets $y = \{y_i\}_{i=1}^n$ (e.g., sequences of forces, temperatures, or wear increments) that are conditionally independent given θ , the likelihood factorises as

$$p(y | \theta) = \prod_{i=1}^n p(y_i | \theta), \quad 2.8$$

which forms the basis for common observation models and numerical inference techniques applied in machining research. Common likelihood choices include Gaussian noise models for metrology signals, lognormal models for nonnegative measurements, or state-space formulations when serial correlation is present. For experiments across multiple operating conditions (tool types, cutting speeds), hierarchical priors allow pooling of information while retaining condition-specific deviations, improving estimation under data sparsity.

Closed-form posteriors are rare in realistic machining applications, and numerical approximations are therefore standard. Markov Chain Monte Carlo (MCMC) methods generate

dependent samples from $p(\theta \mid y)$ under broad conditions. Among these, the No-U-Turn Sampler (NUTS)—an adaptive Hamiltonian Monte Carlo scheme—avoids manual trajectory tuning and offers efficiency in moderately high dimensions with correlated posteriors. For sequential data streams, particle (sequential Monte Carlo) methods and Bayesian filters provide online updates at controlled computational cost (Salehi 2019).

Posterior samples enable *posterior predictive* inference for any derived quantity z (e.g., a future force value, the time to reach a wear threshold, or a surface integrity metric), via

$$p(z \mid y) = \int p(z \mid \theta) p(\theta \mid y) d\theta. \quad 2.9$$

Uncertainty can be summarised by credible intervals and decision-relevant probabilities, such as the probability that flank wear exceeds a critical limit before a scheduled tool change. Routine posterior predictive checks (PPC) compare replicated data from the model against observations to diagnose lack of fit (e.g., systematic bias or dispersion mismatch).

Bayesian methods have been successfully applied to tool condition monitoring and life prediction. Examples include naïve Bayes classification of wear states from multisensor features (Karandikar & McLeay et al. 2015), dynamic Bayesian networks fusing force, temperature, and vibration for real-time condition inference, and online updating of tool-life models in high-speed cutting. Within hybrid digital-twin frameworks, Bayesian posteriors provide probabilistic input distributions (e.g., for wear or friction coefficients) to finite element models, while simulator outputs can inform priors or likelihoods. This bidirectional exchange supports uncertainty-aware process design, parameter calibration, and predictive control of machining operations.

2.6 Summary and Research Gap

Turning imposes coupled thermo–mechanical loads across the primary, secondary, and tertiary deformation zones. These loads, determined by process parameters (v_c, f, a_p) , tool macro- and micro-geometry $(r_e, r_\beta, \gamma, \alpha)$, lubrication/coatings, and progressive flank wear VB , govern near-surface microstructure, residual stress, and topography, i.e., *surface integrity*.

The literature has established (i) the physics of chip formation and tribology, (ii) process and structure relations affecting surface integrity, (iii) metrology for topography, microstructure, hardness, and residual stress, and (iv) modelling approaches from empirical regressions to FE simulations with advanced constitutive and contact laws, as well as first probabilistic treatments of uncertainty. Despite this progress, several limitations remain:

- (a) **Fragmented, single-metric validation.** Most validation is restricted to cutting forces, with few studies including tool-side temperature or strain gradients. Multi-sensor, time-

resolved validation across wear states (VB) and process regimes (v_c), together with uncertainty-aware performance metrics, is still rare.

- (b) **Under-identified wear–boundary condition link.** The causal chain $VB \rightarrow$ contact length/pressure $\rightarrow$ friction regime and heat partition $\rightarrow$ DRX kinetics remains insufficiently quantified. Few FE studies update tool geometry and boundary conditions consistently with measured wear or establish calibrated mappings from VB to contact/thermal parameters using in-situ data.
- (c) **Uncalibrated contact/heat-transfer uncertainty and lack of propagation.** Stick–slip and BUE behaviour along r_β and uncertain thermal contact conductance are major error sources. Inverse identification against spatially resolved temperature data is uncommon, and uncertainty is seldom propagated to surface-integrity predictions. Predictive intervals for UFG/DRX layer properties are therefore absent or uncalibrated.

Therefore, a unified and production-relevant framework is required that (i) constrains physics-based simulations with *tool-integrated, spatially resolved* temperature and wear measurements, (ii) predicts *DRX/UFG* through physically anchored microstructure kinetics driven by FE fields $(\varepsilon, \dot{\varepsilon}, T, t)$, and (iii) quantifies and propagates uncertainty to support early, risk-aware parameter selection and tool-change decisions. The next chapter formulates the corresponding research objectives and outlines a methodology to address these gaps.

3 Research Goals and Approach

This chapter defines the research goals, methodological approach, and scope of the present work. The overarching aim is to develop and experimentally validate a physics-informed and uncertainty-aware framework for predicting wear-dependent surface integrity in hard turning. During turning, the workpiece near-surface is subjected to severe thermo-mechanical loading that can induce dislocation accumulation, dynamic recrystallisation (DRX), and ultrafine-grained (UFG) layer formation. Conventional finite-element models describe chip formation and local loading but rarely connect these fields to microstructural evolution under changing tool-wear conditions. In addition, process variability and measurement uncertainty limit purely deterministic wear predictions. These challenges are addressed by combining microstructure-based finite-element simulations, tool-integrated thin-film sensing, and Bayesian tool-wear estimation.

3.1 Research Goals

The overall goal is to relate the process conditions and the current tool-wear state to the resulting UFG-layer depth as a microstructural indicator of surface integrity. The following specific goals are pursued:

1. **Experimental characterisation of local process loading:** Obtain spatially and temporally resolved temperature, force, strain, and strain-rate data for the calibration and validation of the numerical models.
2. **Microstructure-based prediction of grain refinement:** Develop and validate a finite-element-based framework that relates local thermo-mechanical loading histories to DRX and UFG-layer formation.
3. **Wear-dependent prediction under realistic turning conditions:** Extend the modelling framework from two-dimensional orthogonal cutting to three-dimensional turning and quantify the influence of process parameters and progressive tool wear on the UFG-layer depth.
4. **Uncertainty-aware tool-wear estimation:** Develop a Bayesian framework for sequential estimation of the tool-wear state while accounting for measurement and model uncertainty.
5. **Process-accompanying surface-integrity prediction:** Combine the FE-based microstructure predictions with Bayesian wear estimation to obtain probabilistic predictions of the wear-dependent UFG-layer depth.

3.2 Research Approach

A hybrid physics-informed workflow is employed to achieve these goals. Experimental measurements provide data for model calibration and validation. Validated FE simulations generate time-resolved thermo-mechanical loading histories, which are transferred to a microstructure model in post-processing. Bayesian inference is used to update the estimated tool-wear state as new measurements become available. Finally, the probabilistic wear estimates are combined with an interpolated FE database to predict the corresponding UFG-layer depth.

The workflow comprises:

1. **Tool-integrated sensing and experimental characterisation:** Thin-film sensors are designed, fabricated, and calibrated to measure temperatures close to the tool–chip contact zone. The measurements are combined with dynamometry, high-speed imaging, and digital image correlation for FE-model calibration and validation.
2. **Finite-element modelling in 2D and 3D:** Two-dimensional orthogonal cutting models are used for mechanism studies and model validation. A three-dimensional turning model represents realistic cutting conditions and discrete tool-wear states. The simulations provide histories of strain, strain rate, and temperature in the workpiece near-surface.
3. **Microstructure prediction:** The FE loading histories drive a dislocation-density- and strain-accumulation-based model in post-processing to predict DRX and UFG-layer.
4. **Bayesian wear estimation:** Tool-wear progression is inferred using a Bayesian model and NUTS–MCMC. Prior information is sequentially updated with new wear measurements, yielding probabilistic trajectories of the flank-wear state, $VB(t)$.
5. **FE database and fast prediction:** A database is generated over the process and wear parameters (v_c, f, a_p, VB) . Interpolation provides continuous predictions between the simulated operating points. Posterior samples of $VB(t)$ are mapped onto this database to obtain probabilistic predictions of UFG-layer depth.

Scope and limitations:

The work focuses on UFG-layer depth as the primary microstructural indicator of surface integrity. Residual stresses are available from the FE simulations but are not systematically calibrated or validated. Hardness is used only as supporting experimental evidence and is not treated as an independent prediction target. Phase transformations and grain growth are not explicitly modelled, and all experiments are conducted under dry cutting conditions. The resulting open-loop framework provides a basis for process-accompanying soft-sensor applications and future closed-loop control.

4 Materials and Methods

This chapter presents the materials, experimental configurations, and analytical approaches employed to investigate microstructural evolution and surface integrity in the turning process. The first section introduces the selected workpiece material and cutting tools. This is followed by the design and fabrication of custom thin-film sensors for in-process measurement of tool–workpiece interactions. The experimental setups are then detailed, with emphasis on reproducing realistic machining conditions while ensuring controlled variation of thermo–mechanical loads. These experiments provide both benchmark data for validation and operating conditions for sensor testing. The modelling framework is based on finite element simulations of chip formation, incorporating frictional contact, heat generation, tool wear, and microstructural changes. Model calibration and validation are addressed with respect to their predictive accuracy for surface integrity metrics. Finally, a probabilistic framework for tool-wear progression is introduced, in which sensor signals are assimilated within a Bayesian inference scheme. This enables sequential wear estimation, uncertainty quantification, and predictive analysis of surface integrity outcomes under realistic machining conditions.

4.1 Workpiece Material

The workpieces investigated in this study were machined from AISI 4140 steel (42CrMo4, quenched and tempered), supplied as cylindrical blanks with a diameter of 50 mm. The material was austenitised at 850 °C in a vacuum furnace, quenched in oil, and subsequently tempered. Although several tempering conditions were provided by the supplier, all experiments in this thesis were carried out using material tempered at 650 °C for 60 min, followed by air cooling. The nominal chemical composition, as provided by the supplier, is listed in Table 4.1. In this condition, the steel exhibited a yield strength of at least 880 MPa and a tensile strength of approximately 970 MPa.

The resulting microstructure was characterised by optical microscopy after mechanical polishing and Nital etching. At the surface, the material predominantly consisted of tempered martensite with a minor fraction of bainite. Representative micrographs of the tempered state are shown in Figure 4.1. Microstructural characterisation was performed both before and after machining, with emphasis on the surface and subsurface layers. Further analytical techniques are described in Section 4.2.

Table 4.1: Chemical composition of AISI 4140 steel in weight percent (supplier data).

C	Si	Mn	P	S	Cr	Mo	V
0.40	0.23	0.74	0.016	0.027	1.04	0.20	0.007

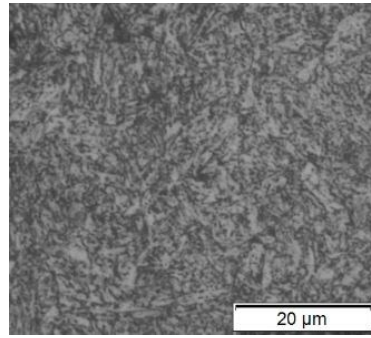


Figure 4.1: Microstructure of AISI 4140 after tempering at 650 °C. All machining experiments presented in this thesis were performed in this heat-treatment condition.

4.2 Surface Integrity Characterisation Techniques

The influence of machining on the near-surface material state was investigated using a set of complementary experimental techniques. Dislocation density was evaluated by X-ray diffraction (XRD) through line-broadening analysis. Strain evolution during selected tests was monitored in-situ using digital image correlation (DIC). Focused ion beam combined with scanning electron microscopy (FIB/SEM) was employed for high-resolution microstructural analysis of the affected zones. Mechanical response was quantified by microhardness testing across the surface and subsurface. Finally, optical microscopy was used to assess surface morphology and etched microstructural features.

4.2.1 Lattice Distortion Analysis via X-ray Diffraction

X-ray diffraction (XRD) was employed to assess subsurface lattice distortions and to estimate dislocation densities in AISI 4140 workpieces before and after machining. Only line-broadening analysis was considered; residual stress determination was outside the scope of this work. The X-ray diffraction measurements were performed at the Institute for Applied Materials (IAM), Karlsruhe Institute of Technology, under the supervision and with the support of Prof. Alexander Kauffmann, using a Bruker D2 Phaser with Cu $K\alpha$ radiation (30 kV, 10 mA). Diffraction patterns were recorded with a LynxEye line detector, using a step size of 0.01° in 2θ and an accumulation time of 384 s per step.

Peak broadening arising from lattice strain was analysed using the Williamson–Hall (WH) method. Within the Williamson–Hall framework, the slope of the linear trend is proportional to the root-mean-square microstrain, while the intercept at $S = 0$ is inversely related to the volume-weighted crystallite size. The broadening in reciprocal space is expressed as

$$\Delta S = \frac{k_s}{d} + \epsilon S, \quad 4.1$$

where ΔS denotes the broadening of the full width at half maximum (FWHM), d is the domain size, ϵ the lattice strain, and $k_s \approx 0.9$. This formulation enables the separation of strain-induced and size-induced contributions to diffraction peak broadening. The scattering vector was calculated as

$$S = \frac{2 \sin \theta}{\lambda}. \quad 4.2$$

Dislocation densities were estimated from the slope of the WH plots using the Williamson–Smallman relation

$$\rho = \frac{\epsilon^2}{b^2}, \quad 4.3$$

where b is the Burgers vector. For reference, the IAM materials database reports dislocation densities in the range of $(0.8\text{--}1.0) \times 10^{15} \text{ m}^{-2}$ for the quenched-and-tempered condition of AISI 4140. These values provide a baseline for interpreting machining-induced lattice distortions. Grain-size effects were neglected, as the X-ray coherence length ($\sim 1 \mu\text{m}$) is significantly smaller than the bulk grain size. To account for elastic anisotropy in BCC steels, both classical and E_{hkl} -normalised Williamson–Hall plots were evaluated. To illustrate the analysis procedure, Figure 4.2 presents exemplary diffraction patterns and Williamson–Hall evaluations for AISI 4140 obtained from the IAM materials database.

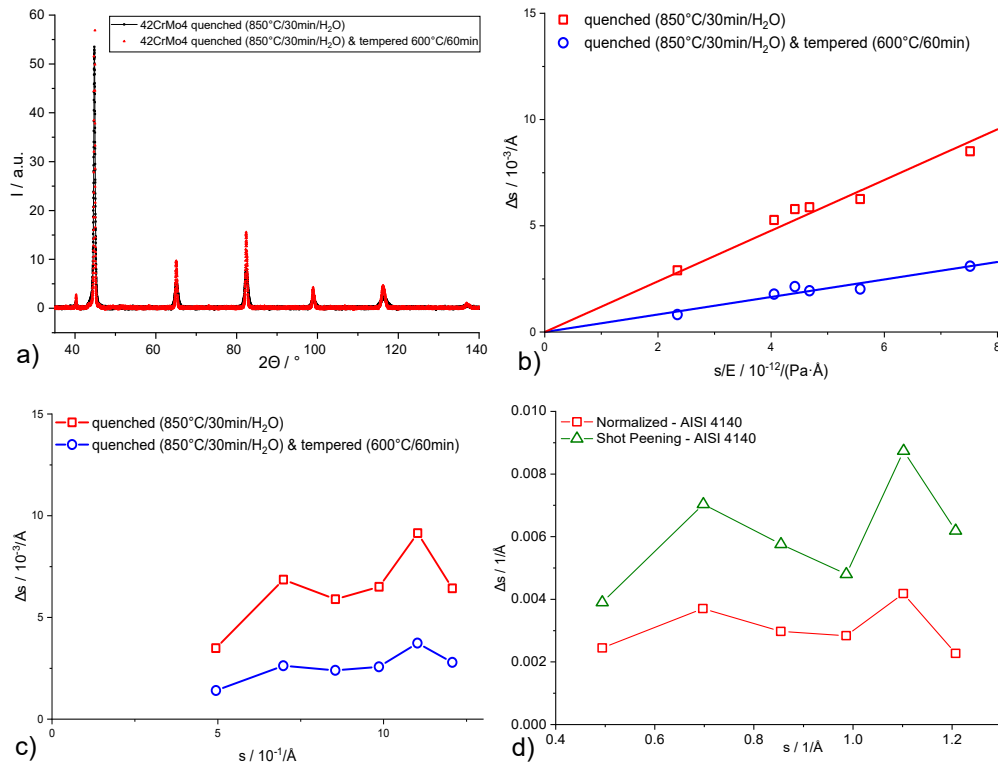


Figure 4.2: Exemplary X-ray diffraction analysis of AISI 4140: (a) diffraction patterns of quenched and tempered states, (b) E_{hkl} -normalized Williamson–Hall plot, (c) Williamson–Hall plot, (d) comparison of normalized and shot-peened samples.

4.2.2 In-situ Strain Field Measurement via Digital Image Correlation

In-situ surface deformation fields were measured using high-speed Digital Image Correlation (DIC) during linear orthogonal cutting, following the experimental procedure established at the University of Kentucky, with the support of Prof. Julius Schoop. DIC provides full-field displacement maps by tracking the motion of a high-contrast speckle pattern across successive high-speed images. A reference frame $I_0(x, y)$ is correlated with each deformed frame $I_t(x, y)$ using subset-based cross-correlation, such that the displacement field $\mathbf{u}(x, y) = (u, v)$ minimises the grayscale residual in each interrogation window,

$$\Delta I = I_t(x + u, y + v) - I_0(x, y). \quad 4.4$$

Spatial differentiation of the displacement field yields the in-plane strain components ε_{xx} , ε_{yy} , and ε_{xy} , which together form the surface strain tensor under the plane-strain conditions characteristic of orthogonal cutting. High-speed imaging was performed using a Photron SA-Z 2001K camera operating at 100 000 fps with an exposure time of 159 ns. A Mitutoyo M Plan APO 20 $\times$ long-working-distance objective provided the required magnification, while a coaxial Heliolux source combined with high-intensity LEDs ensured uniform illumination. A molybdenum-based speckle pattern was applied to the workpiece surface, and the field of view of 640 $\times$ 640 pixels corresponded to a physical scale of approximately 2 μm /pixel.

All correlation calculations were conducted using the `ncorr` toolbox for MATLAB[®] (Blaber & Adair et al. 2015). Under the selected subset and step parameters, the displacement resolution was approximately 0.01 pixels (roughly 20 nm), resulting in strain uncertainties of 8–10% and strain-rate uncertainties of up to $\pm 15\%$ in regions of high deformation gradient.

Strain rates were obtained by temporally differentiating the strain tensor using a central-difference approximation with a time increment of $\Delta t = 10 \mu\text{s}$:

$$\dot{\varepsilon}_{ij}(t) = \frac{\varepsilon_{ij}(t + \Delta t) - \varepsilon_{ij}(t - \Delta t)}{2 \Delta t}. \quad 4.5$$

This allowed resolving dynamic deformation processes within the primary shear zone, where characteristic strain-rate magnitudes are on the order of 10^4 – 10^5 s^{-1} .

Because DIC provides only in-plane strains, the equivalent von Mises strain was evaluated using the standard 2D plane-strain formulation,

$$\varepsilon_{\text{eq}} = \sqrt{\frac{2}{3} [(\varepsilon_{xx} - \varepsilon_{yy})^2 + \varepsilon_{xx}^2 + \varepsilon_{yy}^2 + 3 \varepsilon_{xy}^2]}, \quad 4.6$$

where $\varepsilon_{zz} = 0$ and $\varepsilon_{xz} = \varepsilon_{yz} = 0$ by definition. The equivalent strain rate was computed analogously:

$$\dot{\varepsilon}_{eq} = \sqrt{\frac{2}{3} [(\dot{\varepsilon}_{xx} - \dot{\varepsilon}_{yy})^2 + \dot{\varepsilon}_{xx}^2 + \dot{\varepsilon}_{yy}^2 + 3\dot{\varepsilon}_{xy}^2]}. \quad 4.7$$

From the full-field strain and strain-rate tensors, the following machining-relevant quantities were extracted: maximum in-plane strains ε_{xx} and ε_{yy} ; shear strain $2\varepsilon_{xy}$ and shear strain-rate $2\dot{\varepsilon}_{xy}$; equivalent strain ε_{eq} and equivalent strain-rate $\dot{\varepsilon}_{eq}$; shear angle ϕ determined from the orientation of the dominant shear band; chip–tool contact length l_c ; chip compression ratio; and spatial strain gradients along the primary shear zone.

The complete experimental workflow, including surface preparation, speckle patterning, high-speed imaging, correlation, and strain reconstruction, is illustrated in Figure 4.3.

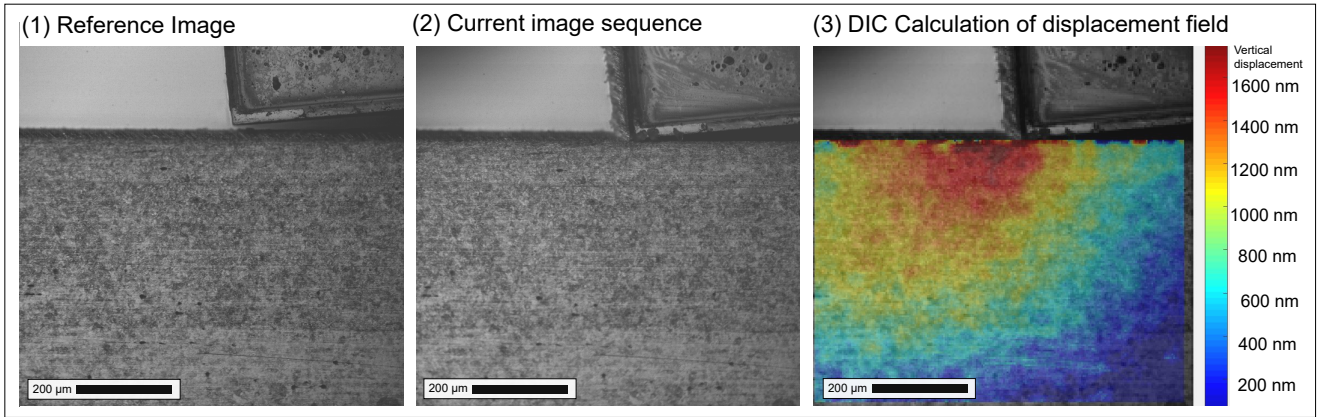


Figure 4.3: Workflow for Digital Image Correlation (DIC) during linear orthogonal cutting.

4.2.3 Microstructural Characterisation and Surface Hardness Profiling

The microstructural changes in the near-surface region of the machined AISI 4140 workpieces were characterised using a dual-beam Focused Ion Beam (FIB) system combined with Scanning Electron Microscopy (SEM). The objective was to identify machining-induced effects such as grain refinement, severe plastic deformation (SPD), and microstructural recovery, as well as to relate these phenomena to local mechanical properties. Although the main emphasis of this work is on the formation of refined and ultrafine-grained (UFG) surface layers, occasional signatures of recovery were also observed in the transition region beneath the severely deformed zone. In FIB/SEM imaging, such recovery is indicated by reduced channeling contrast and smoother grain interiors compared with the adjacent SPD layer, suggesting partial rearrangement or annihilation of dislocations. In the present study, recovery is therefore only discussed qualitatively, whereas the quantitative analysis focuses on the thickness and morphology of the refined grain layers close to the surface.

All FIB/SEM analyses were carried out at the Laboratory for Electron Microscopy (LEM) at the Karlsruhe Institute of Technology (KIT). The system used was an FEI Strata 400 STEM, equipped with a 30 keV Ga⁺ ion source, an energy-dispersive X-ray spectroscopy unit for chemical mapping, and a scanning transmission electron microscopy (STEM) detector for high-resolution imaging. The system provides spatial resolution better than 10 nm in STEM mode. The ion beam was incident at an angle of 38°, and all vertical measurements were trigonometrically corrected.

Cross-sectional specimens were prepared using Electrical Discharge Machining to preserve the original microstructure. The milling directions were aligned with the cutting direction in turning and orthogonal cutting, thereby capturing the directional effects of plastic deformation. Prior to ion milling, a protective platinum layer was locally deposited via a gas injection system to minimise surface charging and reduce roughness artifacts during imaging.

Microstructural imaging was performed using Ion-Induced Channeling Contrast (IICC), a technique that exploits contrast variations caused by ion beam scattering as a function of crystal orientation, strain, and grain boundaries. The layered structure as refined grains near the surface, a zone of SPD grains, and undeformed bulk material; was clearly distinguishable.

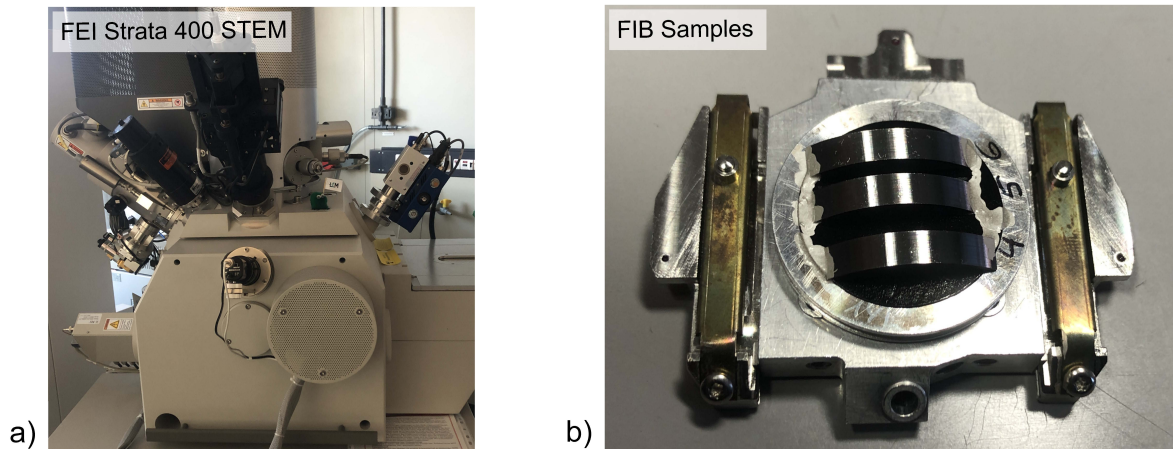


Figure 4.4: a) Dual-beam FIB/SEM system (FEI Strata 400 STEM); b) Mounted FIB samples on the sample holder for cross-sectional milling.

As there is currently no standardised procedure for characterising surface microstructures following machining, the methodology adopted in this work follows the approach proposed by González & Plogmeyer et al. (2020). The segmentation and grain size evaluation were performed using the open-source software ImageJ with the *Trainable Weka Segmentation* plugin (Arganda-Carreras & Kaynig et al. 2017). This tool allows for supervised machine learning-based classification of grain boundaries and enables quantitative image analysis of FIB micrographs. To quantify the thickness of the refined layers, the parameter $z_{gs < X}$ is introduced. It denotes the thickness (in μm), measured orthogonally to the machined surface,

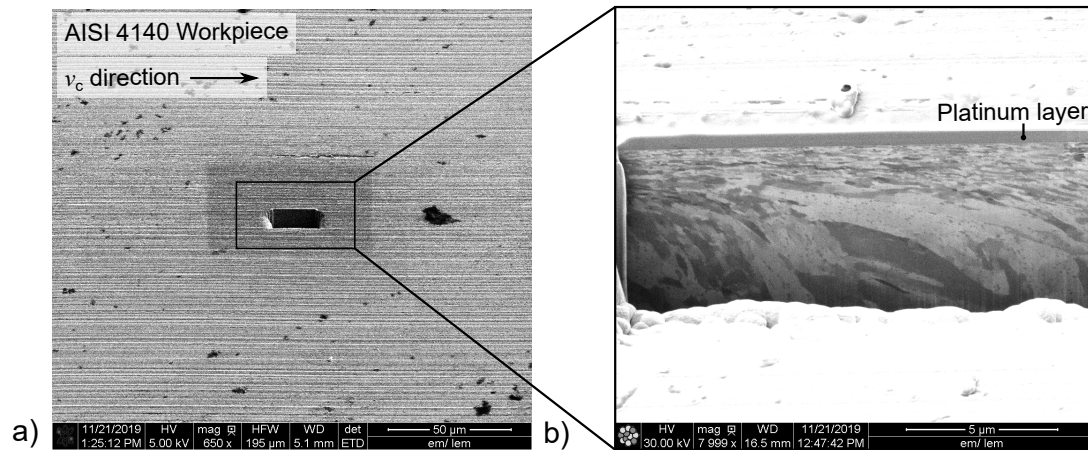


Figure 4.5: a) Cross-section milled by FIB after orthogonal cutting; b) Ion-Induced Channeling Contrast (IICC) image showing surface grain refinement, severe plastic deformation (SPD) layer, and bulk microstructure.

within which more than 95% of the grain diameters are smaller than a specified value X . Each FIB image was analysed at three different positions, and the average value was calculated. An example of the FIB-based microstructural segmentation is shown in Figure 4.6, illustrating the graded surface layers formed during orthogonal cutting.

- **Section I:** Topmost layer subjected to severe plastic deformation (SPD), grain phase transformations, and steep thermal gradients. These effects result in dynamic recrystallisation and the formation of an ultrafine-grained (UFG) structure, where more than 95% of the grain diameters are smaller than 100 nm.
- **Section II:** A subsurface microcrystalline sheared layer with grain sizes below 1 μm in over 95% of the observed area. This indicates significant structural refinement beneath the UFG zone.
- **Section III:** A transition region between the refined surface and the bulk material. This zone is characterised by plastically deformed grains without complete recrystallisation.

For surface hardness profiling, cross-sectional samples from orthogonal cutting and turning experiments were prepared by EDM and embedded in circular mounts using a two-component epoxy resin. The samples were subsequently ground, polished, and etched with an oxide polishing suspension to reveal the surface microstructure prior to indentation. Vickers micro-hardness measurements were carried out using a Qness Q10 tester (Figure 4.7). A low test load of 5 g (HV 0.005) was selected to resolve hardness variations within surface-modified layers thinner than 10 μm. Indentations were spaced at least 5 μm apart to prevent overlap, and a minimum of five measurements were performed per depth level to ensure statistical reliability.

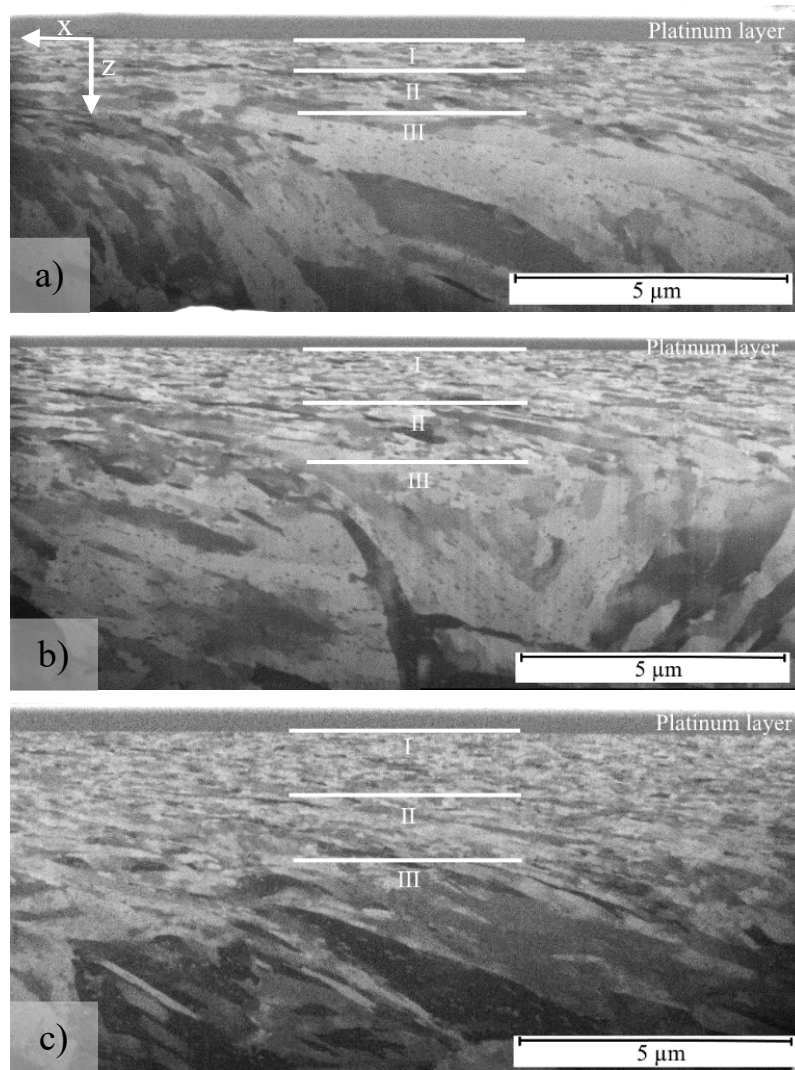


Figure 4.6: FIB image of cross-sections obtained after orthogonal cutting process using: a) uncoated, b) Al_2O_3 -coated, and c) $\text{CrVN} + \text{Al}_2\text{O}_3$ -coated tools. Cutting conditions: $v_c = 150 \text{ m/min}$, $h = 200 \mu\text{m}$. Adapted from González & Plogmeyer et al. (2020).

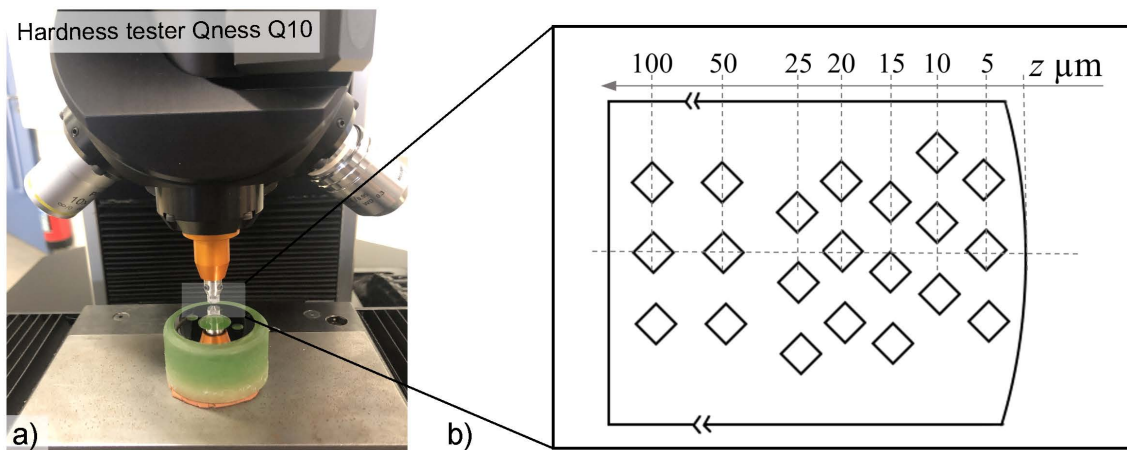


Figure 4.7: a) Microhardness tester (Qness Q10) during operation; b) Representative Vickers indentation pattern on a machined cross-section.

4.3 Optical Tool Wear Characterisation

Tool wear was monitored using a combination of in-situ and ex-situ digital microscopy to track cutting-edge degradation both during and after machining. For in-situ inspection directly at the machine, a Dino-Lite AM7915MZTL USB microscope (10×–140× magnification, 5 MP, 2592×1944 px) with integrated LED lighting was employed, enabling rapid observation without interrupting the cutting process. Detailed ex-situ analyses were subsequently performed using a Keyence VHX-7000 digital microscope (12 MP, 4000×3000 px, 20×–6000× magnification), equipped with a motorised XYZ stage for precise positioning and high-resolution imaging of worn cutting edges. Wear progression was assessed by measuring flank wear land width VB. This combination enabled both real-time monitoring during cutting and comprehensive post-process characterisation of dominant wear mechanisms.

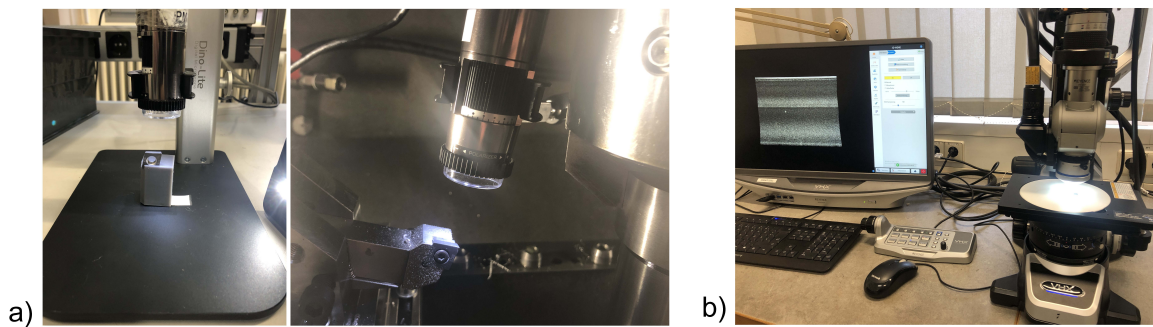


Figure 4.8: Digital microscopy systems: (a) Dino-Lite USB microscope for in-situ monitoring; (b) Keyence VHX-7000 for high-resolution ex-situ inspection of worn cutting edges.

4.4 Thin-Film Sensor-Based Measurement Techniques

Thin-film sensors are highly suitable for in situ monitoring of machining parameters because they withstand extreme environments and provide high spatial resolution. Unlike embedded thermocouples or infrared thermography, which suffer from limited resolution, restricted accessibility, or slow dynamic response, thin-film sensors enable localised, real-time measurement directly at the tool–workpiece interface.

In this work, thin-film systems were employed to measure temperature and wear in the most critical regions of the machining zone. Sensor fabrication, including deposition and photolithographic structuring, was conducted in collaboration with the Fraunhofer Institute for Surface Engineering and Thin Films (IST). The present study focuses on the machining-driven design, placement optimisation, and functional integration of these sensors into production-relevant tooling. The author also developed a compact Raspberry Pi–based data acquisition system tailored for integration in industrial environments.

The following subsections detail the design, positioning strategy, integration challenges, and sensor layout variants. Fabrication techniques and layer calibration procedures are described in prior works (Plogmeyer & González et al. 2020; Plogmeyer & González et al. 2021; González & Plogmeyer et al. 2023).

4.4.1 Sensor Design and Layout Variants

Temperature Sensors

Thin-film temperature sensors were implemented to measure the thermal load in the secondary shear zone—i.e., the tool–chip contact region on the rake face—where heat generation is most intense. Since direct temperature measurement on the dynamically changing work-piece surface is impractical, sensors were strategically placed on the tool side to infer interface temperatures indirectly.

The multilayer thin-film system consists of: (1) an electrically insulating Al_2O_3 base layer (3–5 μm), deposited via Physical Vapour Deposition (PVD) to isolate the sensor from the conductive cemented carbide substrate; (2) a patterned chromium layer serving as the temperature-sensitive element due to its near-linear thermoresistive properties and robust mechanical performance (Biehl & Lüthje et al. 2006); and (3) a protective top layer of Al_2O_3 (up to 3 μm), designed to mitigate wear and exposure to cutting fluids. One known limitation is the low thermal conductivity of the top ceramic layer, which causes a measurable delay between the actual interface temperature and the sensor response. This was addressed through calibration using thermal modelling, incorporating heat-transfer coefficients and layer thicknesses (Plogmeyer & González et al. 2020). Figure 4.9 shows the complete sensor stack and an example layout implemented on an SNGA 190908 insert. Multiple sensor geometries were tested (Figure 4.10), including linear tracks, compact meanders (e.g., 80 $\mu\text{m} \times 80 \mu\text{m}$), and curved layouts. These configurations were chosen to balance spatial resolution, robustness, and signal amplitude. Curved tracks demonstrated higher mechanical reliability under cyclic thermal loads. High-resolution photolithography allowed line widths down to 10 μm and lengths up to 400 μm . Each sensor was designed to achieve a minimum resistance of 50 Ω to ensure measurement precision. Layout variants were adapted to orthogonal cutting inserts and chip-breaker geometries, achieving a placement accuracy of $\pm 10 \mu\text{m}$ (Plogmeyer & González et al. 2021; González & Plogmeyer et al. 2023). For orthogonal cutting applications, sensor placement deviated from conventional corner positioning and was aligned along the tool's cutting edge. This is shown in Figure 4.11, where thin-film sensors are applied to CCMW120404 inserts. Two sensors were placed only 100 μm from the cutting edge, maximising sensitivity while minimising interference with chip formation. Photolithographic precision of $\pm 10 \mu\text{m}$ ensured reliable and reproducible placement (Figure 4.11b).

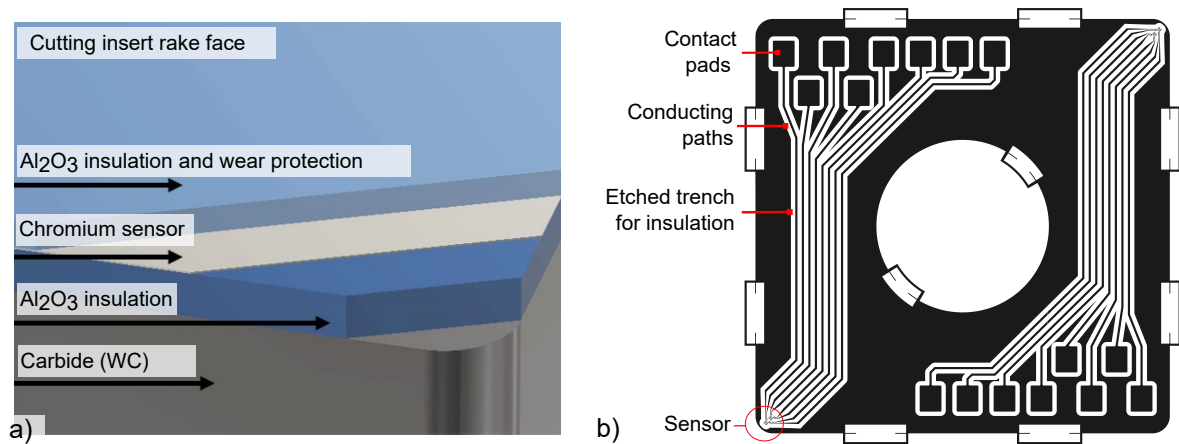


Figure 4.9: Thin-film temperature sensor system: (a) multilayer stack comprising insulation, sensor, and passivation layers; (b) sensor trace layout on an SNGA 190908 tool insert (Plogmeyer & González et al. 2021).

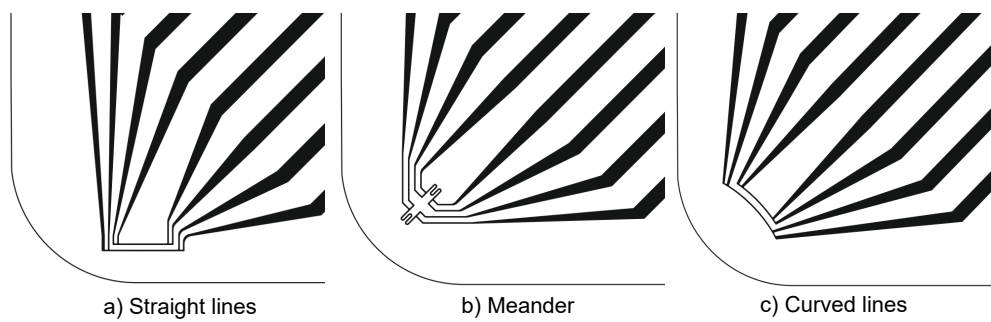


Figure 4.10: Evaluated temperature sensor geometries: (a) straight-line sensors for extended area coverage; (b) compact meander layout for localised temperature fields; (c) curved tracks for robust sensor performance (Plogmeyer & González et al. 2021).

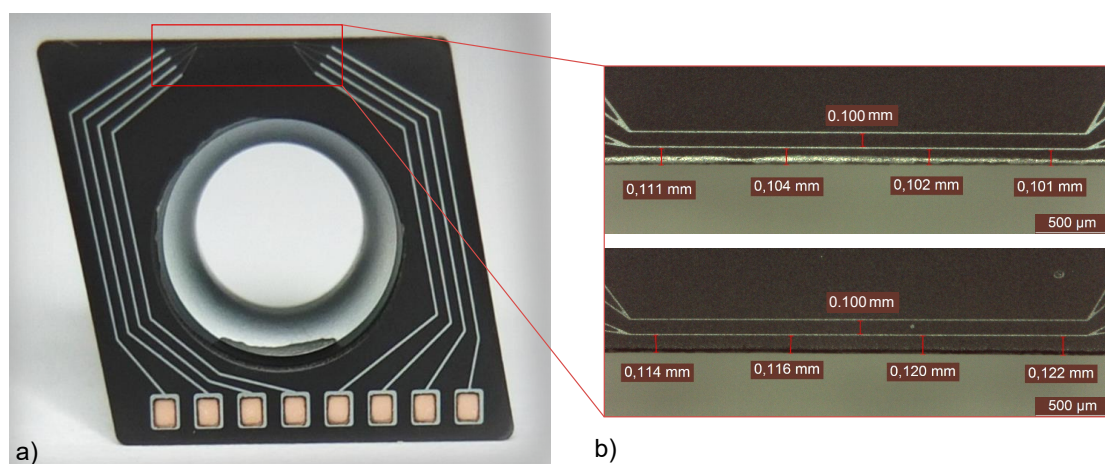


Figure 4.11: Thin-film temperature sensors for orthogonal cutting: (a) sensor placement on a CCMW120404 insert; (b) detail of sensing lines with $\pm 10 \mu\text{m}$ positioning accuracy (Plogmeyer & González et al. 2024).

Integration of thin-film sensors onto complex surfaces, such as cutting inserts with chip breakers and small corner radii, required significant adaptation. Figure 4.12 illustrates a successful implementation on CCMT120404-RP4 inserts featuring such geometries. The sensors were deposited over Tigertec® Silver coating (Walter Tools), which includes an Al_2O_3 wear-protective layer. To ensure electrical insulation, a $1\text{ }\mu\text{m}$ Al_2O_3 layer was applied via PVD, followed by a 200 nm chromium layer patterned through photolithography and wet-chemical etching. A $2\text{ }\mu\text{m}$ Al_2O_3 top layer provided wear protection. Copper-coated contact pads supported either wire bonding or soldering; in this study, shielded wires were soldered to the pads. The final sensor design featured a meander layout measuring $140\text{ }\mu\text{m} \times 140\text{ }\mu\text{m}$. Two sensors, labelled TM1 and TM2, were positioned at distances of $2000\text{ }\mu\text{m}$ and $2250\text{ }\mu\text{m}$ from the cutting edge, respectively. These positions, located directly in front of the chip breaker, were selected to minimise mechanical interference while preserving sensitivity to heat flow within the tool.

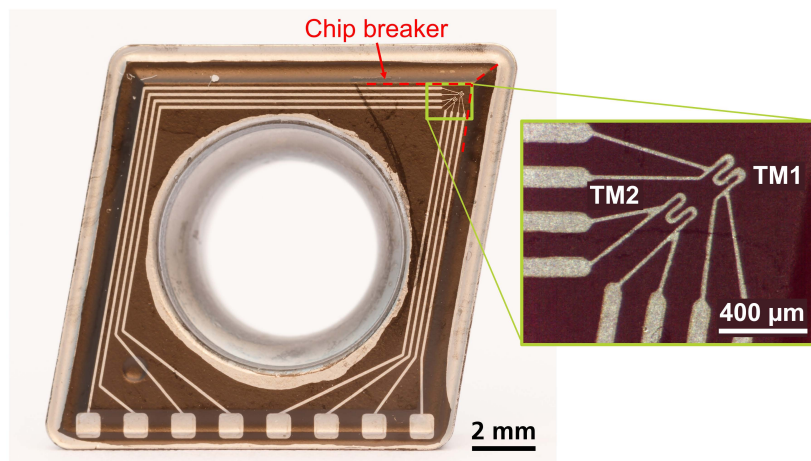


Figure 4.12: Thin-film temperature sensors implemented on a CCMT120404-RP4 insert with chip breaker: sensor placement 2–2.25 mm behind the cutting edge; meander structures protected by a multilayer coating system.

Wear Sensors

To monitor abrasive wear, resistive thin-film tracks were embedded on the rake and flank faces of the cutting insert. As material removal progresses due to crater or flank wear, these conductive paths are sequentially ablated. The resulting discontinuities lead to measurable, stepwise increases in total resistance, which can be used to track the evolution and location of wear. Each conductive path is tailored in width and spacing to generate distinct resistance changes, ensuring resolution without interfering with the cutting process. Figure 4.13 shows three practical configurations implemented on SNGA 190908 inserts: (a) sensors on the rake face for crater wear detection, (b) flank-face sensors for monitoring contact-induced wear on the relief surface, and (c) a corner design capturing wear around the cutting edge radius. This distributed layout enables localised identification of tool degradation during operation.

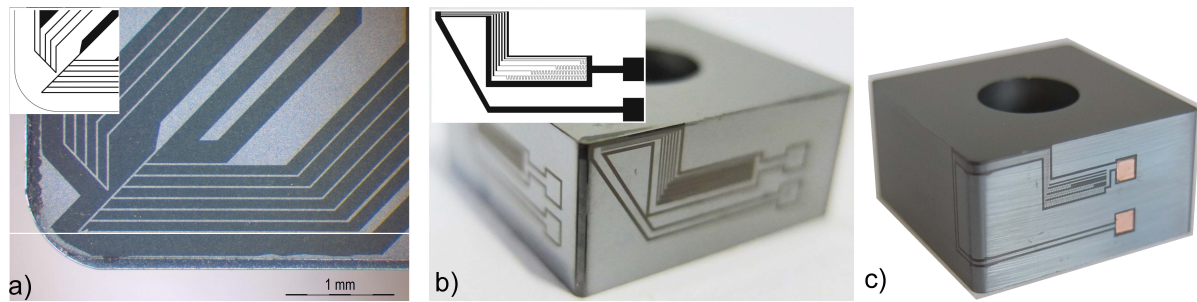


Figure 4.13: Thin-film wear sensor configurations on SNGA 190908 inserts: (a) rake-face sensor for crater wear; (b) flank-face sensor for flank wear; (c) corner sensor. Adapted from (Plogmeyer & González et al. 2020).

4.4.2 Sensor Positioning and Integration Strategy

This section outlines the key stages involved in the fabrication and integration of thin-film sensors used for in situ monitoring of temperature and wear during machining. While the deposition and microstructuring of sensor layers were performed at Fraunhofer IST, the author was responsible for preparing the cutting-tool substrates and conducting the experimental integration and validation of the sensor-equipped tools.

Tool Preparation

To ensure reliable adhesion and long-term stability of the thin-film system, all cutting inserts underwent meticulous surface preparation. The rake and flank faces of cemented-carbide tools were ground using a Buehler planar grinder equipped with diamond abrasive disks, operating at 150 rpm with a constant load of 35 N. The resulting cutting-edge geometry was characterised by a uniform radius of $r_\beta = 5 \mu\text{m}$, while the surface roughness was measured to be below $R_z = 0.1 \mu\text{m}$, as verified by a Mahr Perthometer and a confocal microscope. These conditions minimise topographical defects such as spikes or pinholes, which can compromise the integrity of the insulation layer. Final cleaning was carried out in an ultrasonic bath with acetone and isopropanol to eliminate contaminants before deposition.

Deposition and Structuring

Sensor fabrication commenced with the deposition of a $3.5 \mu\text{m}$ thick aluminium oxide (Al_2O_3) layer by PVD to serve as the electrical insulator between the sensor and the metallic substrate. This was followed by a 100 nm thick chromium layer, selected for its stable thermoresistive behaviour and high adhesion to oxide surfaces.

To define the sensor geometry, a photolithographic process was employed. A photoresist was deposited over the chromium layer, selectively exposed to UV light through a high-resolution mask, and developed to reveal the desired sensor patterns. The exposed chromium regions were removed by wet-chemical etching, leaving behind the functional sensor elements.

To protect the sensor from abrasive wear and chemical attack during machining, a second Al_2O_3 passivation layer ($2\text{ }\mu\text{m}$) was deposited over the patterned chromium structures. Finally, the contact pads were coated with a thin copper layer to facilitate soldering or wire bonding and electrical interfacing.

For inserts with complex geometries, such as chip-breaker structures or sharp edge transitions, electrophoretic deposition (EPD) was used instead of conventional spin or spray coating to apply the photoresist. EPD allows uniform and conformal resist coating even in recessed or irregular areas. The charged resist particles migrate under an applied voltage and deposit on the tool surface, naturally ceasing once full coverage is achieved. This technique enabled the placement of sensor tracks as close as $100\text{ }\mu\text{m}$ to the cutting edge, thus improving thermal sensitivity and spatial resolution. The integration process concluded with visual and microscopic inspection to confirm correct alignment and geometry, prior to sensor calibration and deployment in cutting tests.

Contacting and Calibration

After completion of the thin-film fabrication, electrical connections were established by soldering shielded micro-wires to the copper-coated contact pads. To ensure mechanical stability and resistance to coolant and chip impact during machining, the soldered joints were encapsulated with a thin epoxy layer. This encapsulation step is critical for maintaining signal integrity in harsh process environments and preventing contact failure due to vibrations or debris. Each temperature sensor was individually calibrated to determine its thermoresistive behaviour, which can vary slightly due to differences in fabrication conditions. The calibration procedure involved controlled heating of the sensor-equipped insert inside a laboratory furnace while measuring the output resistance across a range of temperatures. Initial calibrations were limited to a maximum temperature of $170\text{ }^\circ\text{C}$, constrained by the melting point of the soldered contacts used for electrical interfacing. Resistance was measured using a four-wire method to exclude lead resistance, and temperature was recorded with a Pt100 sensor placed directly on the tool rake face using thermally conductive paste.

To overcome the thermal limitations of soldered contacts and extend the calibration range beyond $170\text{ }^\circ\text{C}$, a novel test rig was developed (González & Plogmeyer et al. 2023). In this configuration, the sensorised inserts were placed on a precision-controlled heated aluminium plate and surrounded by metallic shielding to reduce ambient heat losses. Electrical connections were established through spring probes pressed against the contact pads. These were mounted in a custom-designed fixture originally made from PTFE, chosen for its insulating and chemical-resistant properties. However, since PTFE degrades at temperatures above approximately $260\text{ }^\circ\text{C}$, its long-term application at $400\text{ }^\circ\text{C}$ is limited. For sustained high-temperature calibration, alternative materials such as ceramics were considered to ensure

thermal stability. The fixture accommodated twelve spring probes, enabling the simultaneous connection of all three sensors on a single insert. The surface temperature was monitored with a commercial Pt100 sensor placed adjacent to the sensor area. This approach enabled calibrations up to 400 °C with high accuracy and repeatability, while eliminating the risk of solder degradation. The thermoresistive behaviour of each sensor was modelled using a second-order polynomial:

$$R(T) = R_0 \cdot [1 + \alpha \cdot (T - T_0) + \beta \cdot (T - T_0)^2], \quad 4.8$$

where R_0 is the resistance at the reference temperature $T_0 = 0^\circ\text{C}$, and α , β are the temperature coefficients. The average values obtained were $\alpha = 1.0 \times 10^{-3} \text{ K}^{-1}$ and $\beta = 1.2 \times 10^{-6} \text{ K}^{-2}$.

4.4.3 Thermal Conductivity Characterisation

Thermal conductivity (k) is a key material property governing heat dissipation during machining. In the context of thin-film sensor integration, it directly influences the accuracy of measured temperatures, the distribution of heat within the tool and workpiece, and the interpretation of thermal gradients in both experimental and simulation-based studies.

To accurately represent the thermal behaviour of sensor systems, material-specific conductivity values were determined and applied to thermal modelling and sensor calibration procedures. For the Al_2O_3 insulation and passivation layers, experimental characterisation was conducted using the extended 3ω method (Cahill & Katiyar et al. 1994), yielding a thermal conductivity of $k = 1.6 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$ at 25 °C for a 4.4 μm thick film. At elevated temperatures (500–600 °C), values increase moderately to the range of $k = 2\text{--}3 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$, as reported in the literature (Lee & Cahill et al. 1995). This low thermal conductivity, especially compared with metallic films and substrates, enhances the thermal shielding effect of the sensor system. It restricts radial heat dissipation into the tool body and amplifies surface temperature gradients—critical for sensor positioning and thermal resolution. The cemented-carbide substrate (WC–Co), in contrast, exhibits a high thermal conductivity of approximately $k = 120 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$ (Schultrich & Poeßnecker 1988), ensuring rapid lateral heat conduction away from the cutting zone. Chromium-based sensor tracks and CrVN coatings were not measured directly, but reference values from related studies suggest intermediate conductivities between those of oxides and metallic substrates (Tlili & Nouveau et al. 2012).

These values were used as input parameters for finite-element simulations of chip formation and for computing effective interface temperatures during sensor calibration. Their inclusion ensures physical consistency across the experimental and numerical methodologies employed in this study.

4.4.4 Data Acquisition and Operational Deployment

A dedicated data acquisition (DAQ) system was developed by the author for real-time monitoring of resistance-based signals from integrated thin-film temperature and wear sensors. The system is designed for cost efficiency and robustness, enabling reliable operation under industrial machining conditions. It integrates a Raspberry Pi® Model 4B with an MCC118 DAQ HAT and a custom constant-current HAT providing three stable 1.00, mA excitation sources. A four-wire measurement configuration is employed to eliminate lead-resistance effects and ensure accurate resistance measurements during operation.

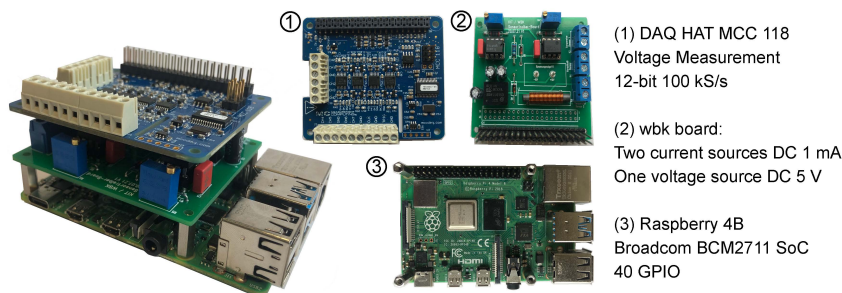


Figure 4.14: Portable Raspberry Pi-based DAQ system for thin-film sensor monitoring: (1) MCC118 DAQ HAT (12-bit, 100 kS/s); (2) custom wbk HAT with three 1 mA current sources; (3) Raspberry Pi 4B as processing and control unit.

During machining, the DAQ system was synchronised with high-speed imaging to ensure temporal alignment of thermal, force, and strain-field data. Temperature signals were calibrated from raw resistance measurements and filtered using a 25, Hz low-pass filter to reduce noise, with both raw and filtered signals retained for analysis (Fig. 4.15a). Tool wear was monitored via resistive tracks, and automated step detection identified discrete resistance increases corresponding to progressive material removal during cutting (Fig. 4.15b).

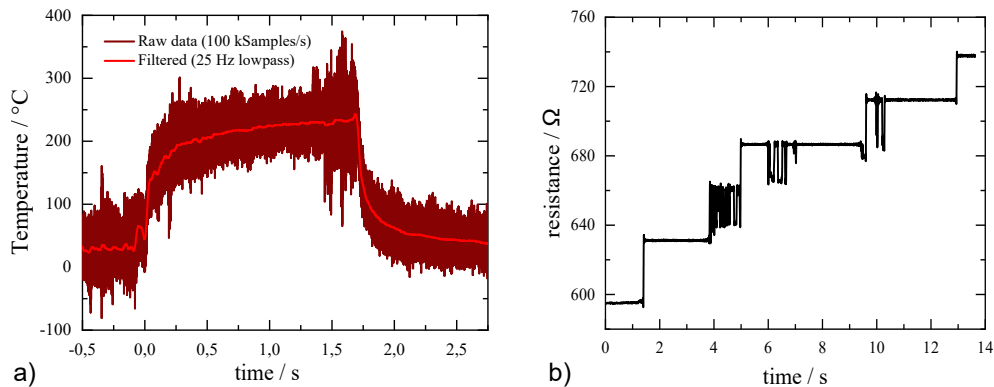


Figure 4.15: Sensor signal acquisition during turning tests: (a) raw and filtered temperature signal; (b) resistance evolution of wear sensors showing discrete jumps corresponding to path breakage (Plogmeyer & González et al. 2020).

4.5 Experimental Setups for Machining Trials

To investigate the effects of machining parameters on the surface integrity of AISI 4140 steel, three complementary experimental setups were employed: (1) linear orthogonal cutting, (2) rotary orthogonal cutting, and (3) longitudinal turning. Each configuration isolates specific aspects of the cutting process, ranging from fundamental chip formation to industrially relevant tool–workpiece interactions. Together, they provide a framework for correlating mechanical and thermal loads with tool behaviour and surface response.

The linear orthogonal setup offers high accessibility for in situ optical observations of chip formation. The rotary orthogonal configuration enables extended engagement times under orthogonal conditions, suitable for thermal and wear studies. The longitudinal turning setup reproduces industrially relevant cutting conditions and facilitates comprehensive integration of thin-film sensors. The following subsections describe each setup in detail.

4.5.1 Linear Orthogonal Cutting

Linear orthogonal cutting experiments were performed on a high-precision, ultra-high-speed testbed developed at the Institute for Sustainable Manufacturing (ISM), University of Kentucky. The setup was designed to provide plane strain conditions and high optical accessibility, enabling in situ investigations of material deformation, chip formation, and subsurface strain localisation during finishing operations.

The testbed, presented in Fig. 4.16, comprises a rigid granite base reinforced by a welded steel frame anchored to the facility's foundation. A linear servo motor drives the primary cutting axis (x -direction), achieving velocities up to 4 m/s and accelerations of 5 G, with encoder feedback ensuring nanometric positioning accuracy. Auxiliary servo drives control the orthogonal (y) and vertical (z) axes, providing positioning repeatability within 0.4 μm . A Capto C3 tool holder is mounted on the z -axis to guarantee rigidity and reproducible tool alignment. All experiments were performed under dry cutting conditions at ambient laboratory temperature.

Workpieces made of AISI 4140 were fabricated by EDM, followed by grinding and mirror polishing to eliminate residual stresses (Fig. 4.17). Flatness was critical due to the 30 μm depth of field of the high-speed imaging system. Each specimen had a machining thickness of 3 ± 0.001 mm in the cutting zone and a reinforced central section (6.35 mm) for clamping. Chamfers were introduced at tool entry and exit to minimise stress concentrations and vibrations. Cutting speeds in the range $v_c = 30\text{--}120$ m/min and uncut chip thicknesses $h = 50\text{--}125$ μm were selected to reproduce finishing conditions.

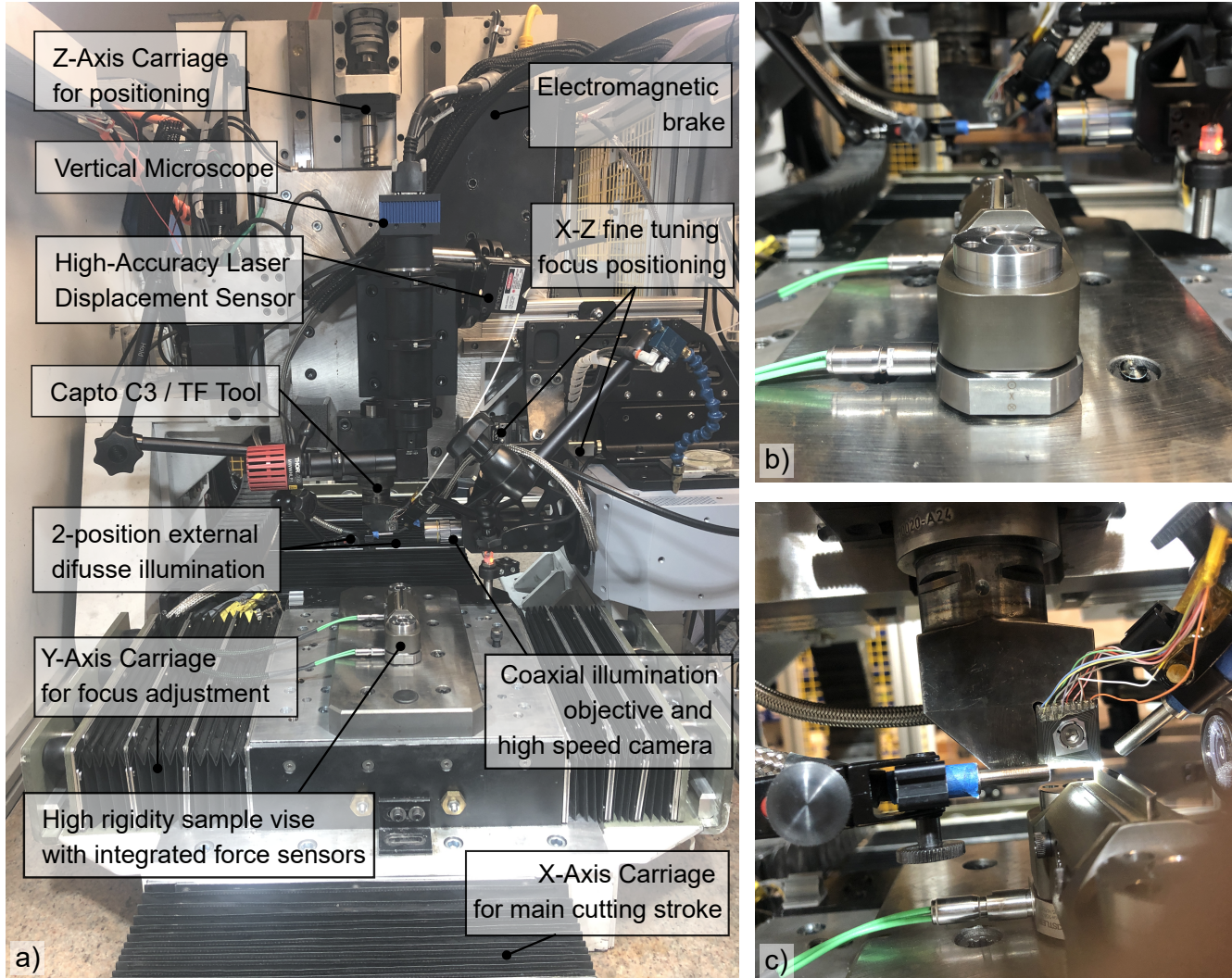


Figure 4.16: Linear orthogonal cutting setup at the University of Kentucky: (a) custom in situ testbed; (b) workpiece fixture with piezoelectric force transducers; (c) cutting tool with thin-film sensors and coaxial illumination.

Cutting forces were measured using two triaxial piezoelectric transducers (Kistler 9027C) mounted beneath the workpiece fixture. Simultaneously, chip formation was recorded with the high-speed imaging system described in Section 4.2.2, enabling time-resolved observation of shear-zone evolution and material flow. Thin-film temperature sensors were integrated into SNGA 190908 uncoated carbide inserts as described in Section 4.4, resulting in a multilayer Al_2O_3 coating with a thickness of $5\ \mu\text{m}$. The inserts featured a rake angle $\gamma = -5^\circ$, clearance angle $\alpha = 5^\circ$, and edge radius $r_\beta = 5 - 10\ \mu\text{m}$. To ensure coplanarity with the workpiece surface, the insert nose was flattened by EDM. Three parallel chromium tracks ($30 \pm 5\ \mu\text{m}$ wide) were patterned on the rake face at distances of $300 \pm 5\ \mu\text{m}$, $400 \pm 5\ \mu\text{m}$, and $500 \pm 5\ \mu\text{m}$ from the cutting edge, each extending 3 mm along the cutting width. Sensor signals were acquired at 100 kS/s and synchronised with the high-speed imaging trigger, ensuring temporal alignment across force, temperature, and strain-field measurements.

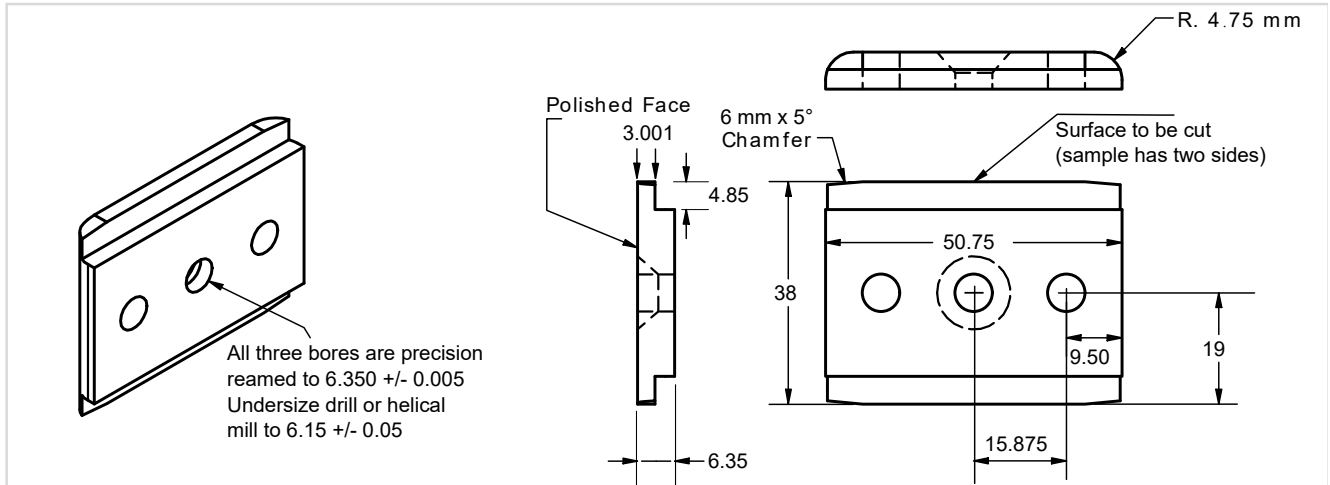


Figure 4.17: Workpiece for linear orthogonal cutting experiments. Designed at the University of Kentucky and manufactured at KIT.

4.5.2 Rotary Orthogonal Cutting

To bridge the gap between simplified orthogonal tests and realistic turning processes, rotary orthogonal cutting experiments were performed on a CNC vertical turning centre (Index V100). This configuration serves as an intermediary setup, combining the geometric simplicity of orthogonal cutting with the thermal and mechanical boundary conditions of conventional turning.

The workpieces were manufactured from quenched-and-tempered AISI 4140 bars and machined into circular specimens with an initial diameter $D_0 = 49$ mm. Each specimen was equipped with a central hole for clamping and two additional radial holes to accommodate hardened pins, ensuring accurate positioning and concentric alignment within the vertical fixture. The specimens were ground to a uniform thickness of 4 mm in the cutting zone and subsequently reduced to a final diameter of $D_f = 30$ mm during machining.

As the diameter decreased ($D_0 \rightarrow D_f$), the effective surface area available for heat dissipation diminished, resulting in a progressive temperature rise. A true thermal steady state is therefore not achieved, which makes this configuration representative of industrial turning, where continuous heat input typically exceeds dissipation and localised gradients persist.

The cutting setup is illustrated in Fig. 4.18a and b. The tool remained stationary while the workpiece rotated and was fed radially along the x -axis. Cutting speeds up to $v_c = 300$ m/min were applied, allowing investigation of thermal phenomena under intensified conditions. Cemented carbide inserts of type CCMW120404 were used, featuring $\gamma = 0^\circ$, $\alpha = 7^\circ$, and an edge radius of $r_\beta = 50$ μ m.

Cutting forces were measured with a Kistler 9257B piezoelectric dynamometer. The inserts were coated via PVD with multilayer thin-film sensors as described in Section 4.4. To capture the thermal response, thermocouples were embedded into both the tool and the workpiece by EDM-drilled cavities. The measurement system comprised three channels: T_t (tool thermocouple), T_w (workpiece thermocouple), and T_{tfs} (thin-film sensor). The thin-film system (Fig. 4.18c) consisted of two resistive lines placed at 100 μm and 200 μm from the cutting edge to resolve steep thermal gradients near the tool–chip interface.

Thermocouple positions are shown in Fig. 4.18d. Signals from the thermocouples were acquired via a USB-TC module and a wireless MSR160 logger installed in the rotating spindle. This configuration enabled synchronised measurement of cutting forces and thermal fields.

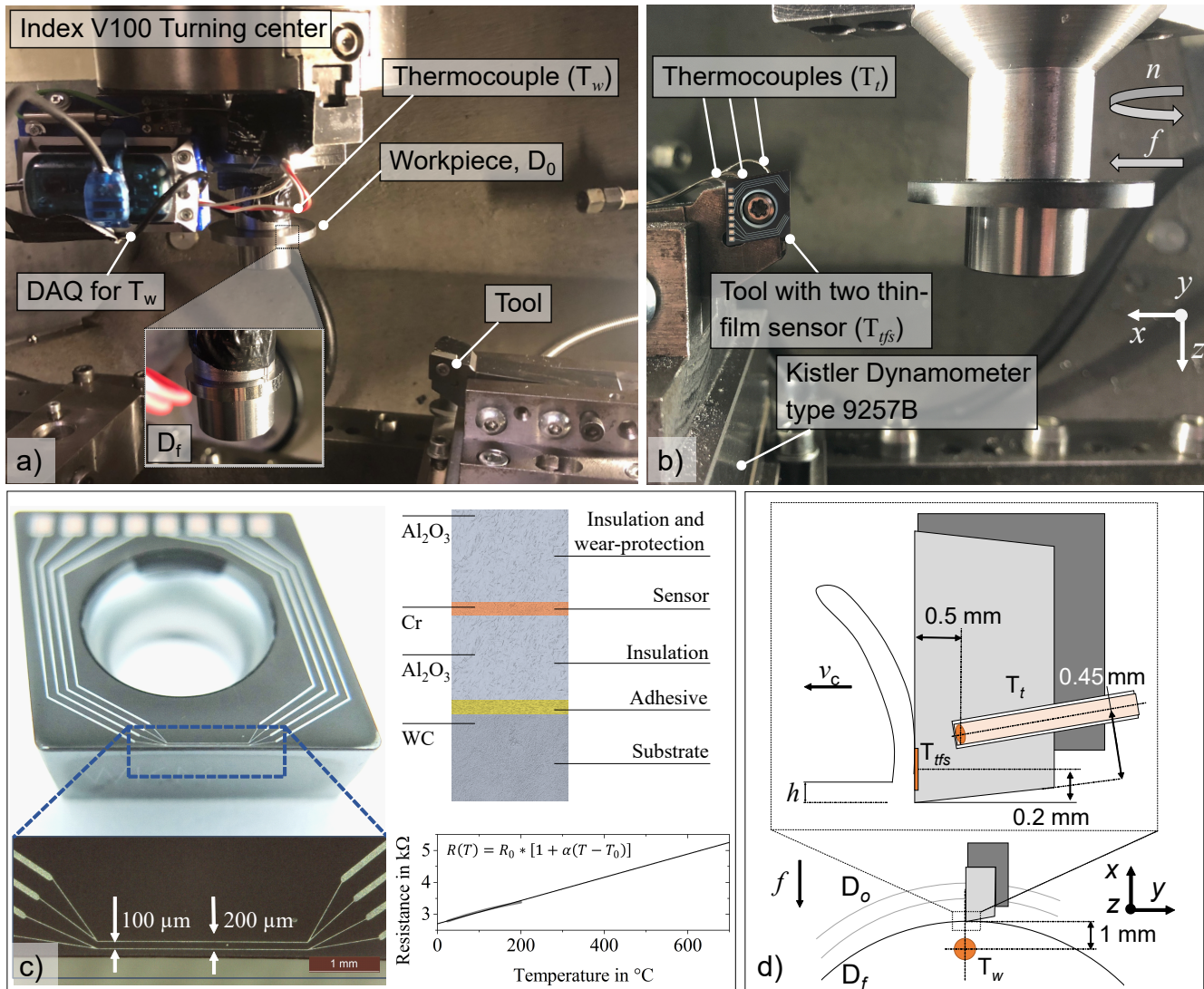


Figure 4.18: Rotary orthogonal cutting configuration on Index V100: (a) CNC vertical turning centre; (b) experimental setup with tool fixed to a piezoelectric dynamometer and rotating workpiece; (c) thin-film sensor stack on cutting insert; (d) sensor layout and thermocouple positions.

4.5.3 Longitudinal Turning

Longitudinal turning experiments were conducted on a horizontal CNC turning centre (Index G200) to study tool–workpiece interactions under industrially representative three-dimensional cutting conditions (Fig. 4.19). This configuration incorporates realistic geometric and operational factors—tool nose radius, chip-breaker design, and progressive tool wear—and was run under dry conditions to emphasise thermal effects, accelerate wear development, and avoid interference with thin-film sensor measurements.

Cylindrical AISI 4140 bars were machined to 50 mm diameter and 300 mm length. Workpieces were clamped in a collet chuck and axially supported by a tailstock. The system allowed uninterrupted longitudinal cuts up to 200 mm. Cutting parameters were varied across the ranges $a_p = 0.3\text{--}1.2$ mm (depth of cut), $f = 0.1\text{--}0.3$ mm/rev (feed), and $v_c = 50\text{--}250$ m/min (cutting speed), covering finishing to semi-roughing regimes.

The cutting tool was mounted on a Kistler® 9119A dynamometric platform integrated in a VDI25 adapter, enabling high-resolution, three-component force measurement directly at the holder. The tool holder was aligned with zero inclination so that recorded components corresponded directly to cutting, feed, and passive forces without trigonometric transformation.

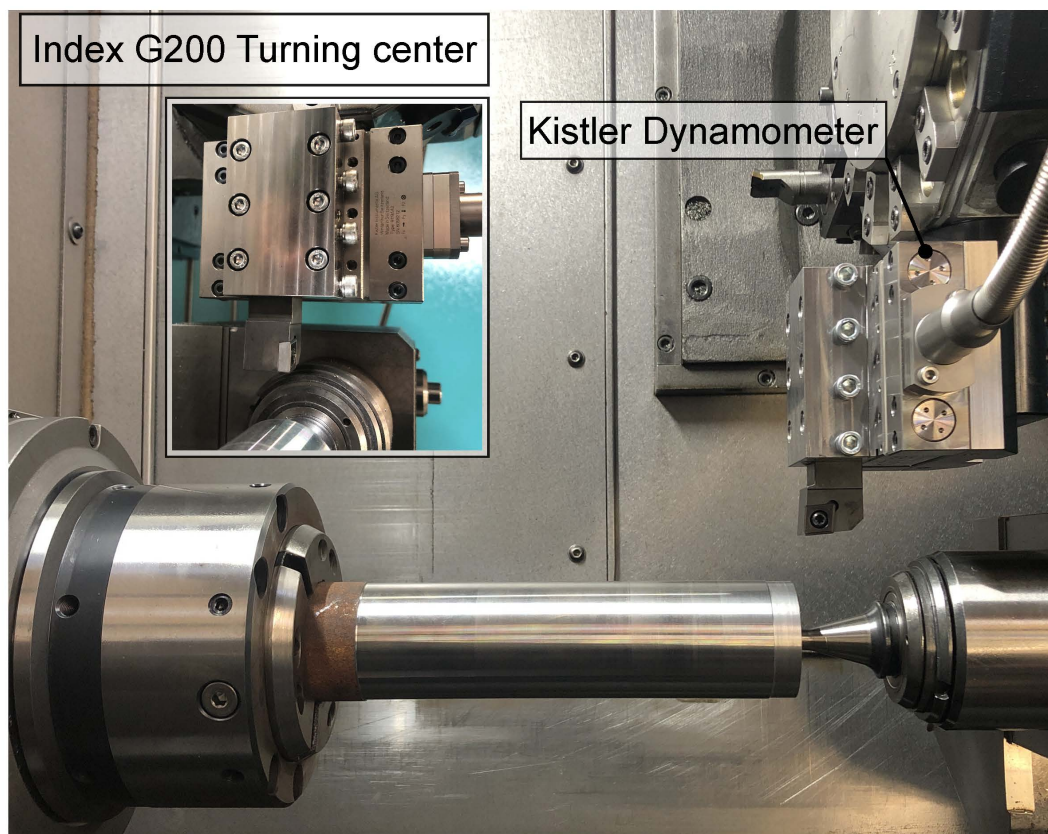


Figure 4.19: Experimental configuration for longitudinal turning on Index G200.

Three coated carbide insert types from Walter AG were used (Fig. 4.20): CCMT120408-FK6, CCMT120408-MP6, and CCMW120408-RK6 (the latter without chip breaker). All inserts shared the following nominal geometry: cutting-edge radius $r_\beta = 45\ \mu\text{m}$, corner radius 0.8 mm, rake angle 7° , clearance angle 7° , and main cutting-edge angle 95° when mounted. Selected CCMT120408-FK6 inserts were instrumented with thin-film sensors for simultaneous measurement of cutting temperature and tool wear (Fig. 4.21).

The temperature sensor consisted of two meander-shaped resistive tracks deposited on the rake face, with the first sensing element positioned 1.675 mm radially from the machined surface. This offset was dictated by the geometric constraints of the PVD process on sharp and curved surfaces.

The wear sensor comprised seven parallel resistive tracks deposited on both flank faces. The first track was positioned 0.100 mm from the cutting edge, with the remaining tracks spaced at 0.050 mm intervals, enabling incremental quantification of abrasive flank wear progression up to 0.450 mm. In addition to the thin-film measurements, an optical wear monitoring system (Dino-Lite USB microscope, see Section 4.3) was employed to record high-resolution images of the cutting edge after predefined cutting lengths. This hybrid approach provided complementary quantitative (sensor-based) and optical data on wear development during the longitudinal turning tests.

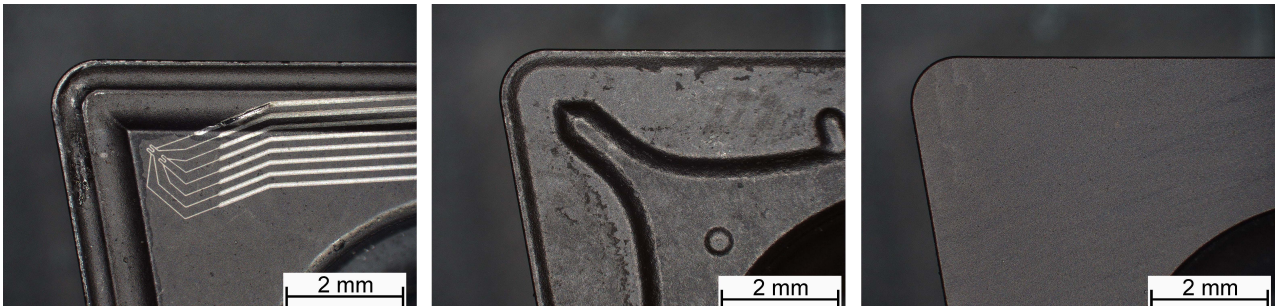


Figure 4.20: Coated carbide inserts used in longitudinal turning experiments: (a) CCMT120408-FK6, (b) CCMT120408-MP6, (c) CCMW120408-RK6.

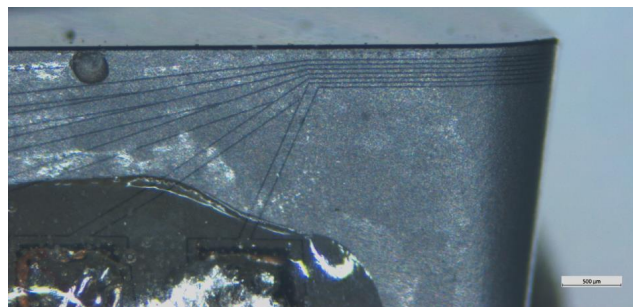
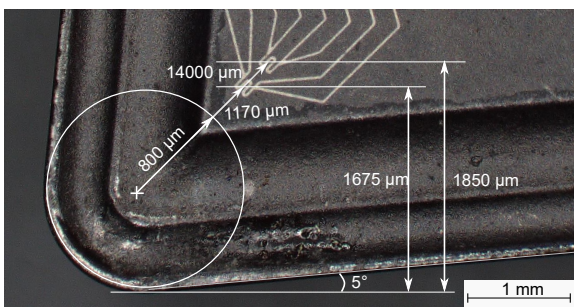


Figure 4.21: Thin-film sensor layout on CCMT120408-FK6 inserts: (a) two meander tracks (TM1 and TM2) for temperature; (b) seven parallel tracks for flank wear detection.

4.6 Finite Element Method

This section presents the implementation of Finite Element Method (FEM) simulations used to model chip formation and subsurface microstructural evolution in machining processes. Both two-dimensional (2D) and three-dimensional (3D) simulations were conducted using the software *Simufact Forming*, with emphasis on mesh adaptation, thermomechanical boundary conditions, and tool–workpiece interaction modelling. The mechanical response of AISI 4140 was described using the Johnson–Cook constitutive model, calibrated through an inverse optimisation procedure based on experimental force measurements. Frictional behaviour at the tool–chip interface was modelled using a combined Coulomb–shear law to account for both sliding and sticking contact regimes. Microstructural changes were evaluated in a decoupled post-processing framework using three distinct models for dynamic recrystallisation (DRX): an empirical Zener–Hollomon formulation, a thermodynamic model based on Helmholtz free energy, and a dislocation density-based approach. Each model was implemented as a standalone subroutine and applied to the FEM output fields (strain, strain rate, temperature). Their predictive capabilities will be compared in section 5.2.3.

4.6.1 2D Chip Formation Model Setup

Two-dimensional orthogonal cutting was modelled under plane-strain conditions using the commercial finite element software *Simufact Forming*. An Arbitrary Lagrangian–Eulerian (ALE) formulation was employed to enable continuous chip separation while maintaining mesh quality in regions of large deformation. This formulation supports iterative remeshing, mesh convection and local refinement, which are essential for accurately resolving the steep strain and temperature gradients that develop in the primary (PDZ) and secondary (SDZ) deformation zones. The workpiece material was described using the Johnson–Cook flow stress model in combination with a decoupled microstructure evolution approach to capture grain refinement beneath the machined surface. The JC model provides the strain, strain-rate and temperature dependence of the flow stress, while post-processing models predict microstructural evolution using these thermomechanical histories. This allows the simulation to represent surface integrity effects under realistic machining conditions without altering the mechanical constitutive behaviour during chip formation.

Simulation Setup and Boundary Conditions

Figure 4.22 illustrates the full simulation domain, which consists of a rigid cutting tool, an elasto-plastic workpiece, an elastic support body, a fixture and a heat sink. In selected simulations, a 5 μm coating layer was included on the tool rake and flank faces to enable consistent calibration against temperature measurements from in-tool thin-film sensors and thermocouples.

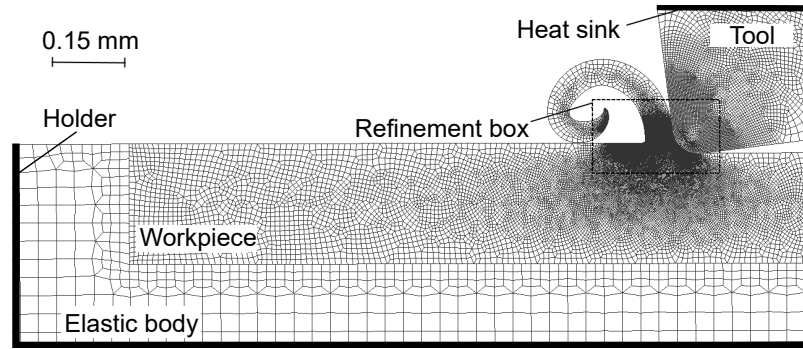


Figure 4.22: 2D simulation setup for orthogonal cutting (González & Segebade et al. 2019).

The workpiece dimensions were set to 0.3 mm (height) and 5 mm (length), ensuring that the effective cutting length (up to 3 mm) and maximum depth of cut (0.2 mm) could be simulated without boundary interactions. The elastic body was dimensioned experimentally to avoid artificial stress reflections. The fixture constrained its outer boundary to avoid rigid-body motion, while the heat sink served as a thermal stabiliser, allowing fine-tuning of the tool temperature field based on experimental data.

Meshing Strategy, contact definitions and temporal discretisation

The mesh was composed of Class 4 quadrilateral elements with bilinear interpolation. Two meshing strategies were applied: Advancing-Front-Quads for the workpiece and tool, allowing boundary-conforming, high-quality elements in the chip formation zone and Quadtree meshing for the elastic body to maintain efficiency. The initial element size was $8\ \mu\text{m}$ and refined *a posteriori* in critical regions using refinement boxes up to $1\ \mu\text{m}$. Dynamic remeshing was triggered when the equivalent plastic strain exceeded 0.4, preventing excessive distortion and allowing the mesh to adapt as the chip formed. Table 4.2 summarises the contact interactions between the simulation components, where **F** denotes a frictional contact interface and **R** denotes a rigidly coupled contact without relative motion.

Table 4.2: Contact settings between simulation components

	Tool	Elastic Body	Workpiece	Fixture	Heat Sink
Tool	—	—	F	R	R
Elastic Body	—	—	R	R	—
Workpiece	F	R	—	—	—
Fixture	R	R	—	—	—
Heat Sink	R	—	—	—	—

Time integration was performed using an explicit time-stepping scheme with an adaptive time increment. The time step was not fixed, but dynamically adjusted based on a kinematic

stability criterion related to the tool advance and local mesh resolution. An adaptive geometric constraint was applied:

$$v_c \Delta t < 0.5 h_{\min}, \quad 4.9$$

where v_c is the cutting speed and $h_{\min}$ is the smallest element size in the mesh. This condition limits the tool advance per increment to half an element, preventing element inversion in the primary deformation zone and ensuring that strain, strain-rate and temperature fields remain accurately tracked during mesh motion.

Quasi-Steady-State Multistage Simulation Strategy

High-fidelity chip formation simulations require extremely fine meshes in the primary and secondary deformation zones to resolve the steep gradients in strain, strain rate, temperature and contact pressure. Directly running a long cutting simulation with such resolution would lead to prohibitively large computational cost. To overcome this, a quasi-steady-state multistage simulation strategy, originally introduced in González & Segebade et al. (2019), was adopted and further refined.

The approach successively builds the thermomechanical state of the system across several stages, each stage inheriting the temperature, strain and stress fields of the previous one. This allows the simulation to approach a physically meaningful steady regime near the tool–chip interface without requiring excessive cutting lengths.

1. **Tool Preheating (Stage 1):** A first cutting simulation of 1.5 mm length is performed using a relatively coarse mesh (8 μm in the workpiece and 5 μm in the tool). To accelerate the thermal equilibration of the tool, its specific heat capacity is artificially reduced by several orders of magnitude (by a factor of 10^{13}). This forces the tool to rapidly adopt the interface temperature dictated by frictional and plastic dissipation at the chip–tool contact. The artificially-enhanced thermal response produces a physically consistent, though computationally accelerated, steady-state temperature profile within the tool. At the end of this stage, the temperature field is extracted and stored for the next step.
2. **Workpiece Thermal Adaptation (Stage 2):** A second, shorter simulation (0.5 mm cutting length) is conducted with a workpiece finer mesh (down to 2.5 μm). The tool is now treated as a thermally inert body, and the temperature field obtained in Stage 1 is imposed and kept fixed. This forces the workpiece to adapt to the preheated tool boundary while avoiding additional numerical transients that would occur if the tool temperature were allowed to evolve again. During this stage, depending on the uncut

chip thickness, one or two chip segments may form, allowing the near-surface workpiece region to reach a thermally stable condition consistent with the cutting process.

3. **Quasi-Steady-State Formation (Stage 3):** The third stage reintroduces the real thermophysical properties of the tool, in particular its actual specific heat capacity. The cutting length is increased to 1.0 mm, and the mesh refined further (minimum element size of 1 μm). The initial temperature and strain fields from Stage 2 are mapped onto the mesh. Because the tool now recovers its realistic thermal inertia, the chip–tool interface temperature evolves in a physically representative manner, resulting in a thermally damped but stable quasi-steady-state. This step is crucial for eliminating the artificial thermal acceleration of Stage 1 while still retaining the preheated state that would be physically present in an actual machining process.
4. **High-Resolution Final Cut (Stage 4):** In the final step, a short segment of high-resolution cutting (0.25 mm) is simulated with a minimum element size of 0.5 μm in the primary shear zone and tool–chip surface contact region. The refined mesh enables accurate resolution of the extreme gradients in strain rate and temperature that drive chip segmentation and subsurface microstructural evolution. The thermomechanical fields inherited from Stage 3 ensure that the system begins this final stage in a quasi-stationary condition, avoiding unrealistic start-up transients. The resulting thermomechanical fields from this stage form the basis for subsequent post-processing with the DRX models.

4.6.2 Friction Model

Building on the theoretical background presented in the state of the art, the tool–workpiece interaction was modelled using the combined Coulomb–shear friction formulation proposed by Agmell et al. (Agmell & Ahadi et al. 2011). This hybrid law explicitly captures the coexistence of sliding and sticking at the tool–chip interface by constraining the interfacial shear stress through two distinct mechanisms: (i) a Coulomb-type term proportional to the local contact pressure, and (ii) a shear strength limit based on the flow stress of the workpiece material. The resulting effective interface shear stress τ_c is expressed as:

$$\tau_c = \min (\mu \sigma_n, m \tau_{\max}) , \quad 4.10$$

where μ is the sliding friction coefficient, σ_n the local normal stress, m the shear limit factor, and $\tau_{\max}$ the material shear strength. The first term represents classical Coulomb friction, which governs the sliding regime at moderate pressures and high chip velocities. The second term imposes an upper bound on the allowable interface shear stress, reflecting the transition

to sticking when the contact pressure is sufficiently high that the workpiece material can no longer sustain additional shear without plastic flow. This formulation overcomes the limitations of a pure Coulomb model, which tends to overpredict interface shear stresses and heat generation in high-pressure contact zones near the cutting edge. The hybrid law naturally reproduces the experimentally observed partition between sticking and sliding observed in dry machining of steels and provides a smoother and more physically meaningful stress distribution along the rake face. Furthermore, since frictional heat generation is directly linked to both sliding velocity and interfacial shear stress, the shear-cap term improves the consistency between predicted and experimentally measured temperature fields.

In this study, the friction parameters were set to $\mu = 0.35$ and $m = 0.70$. Here, μ controls the sliding friction behaviour, while m limits the maximum shear stress to $0.70 \tau_{\max}$, preventing unrealistically high sticking stresses. These values lie within the experimentally validated range for dry machining of AISI 4140 with coated carbide tools, as reported in (Filice & Micari et al. 2007; Arrazola & Özel 2005; Umbrello & Filice et al. 2008). They were selected to ensure compatibility with the dynamometer force measurements, chip morphology observations, and the thermal boundary conditions used during calibration. Compared to the pure Coulomb case, this combined law significantly improves the fidelity of chip thickness, shear plane angle, and temperature predictions, particularly in the high-strain-rate region adjacent to the cutting edge.

4.6.3 Material Model

The material behaviour of the workpiece was described using the Johnson–Cook (JC) constitutive equation, as introduced in Section 2.4.1. The JC formulation is well suited for machining simulations because it captures the three dominant effects governing flow stress under chip formation conditions: strain hardening, strain-rate sensitivity, and thermal softening at elevated temperatures.

As the objective of this chapter is to construct and calibrate a thermomechanically consistent FEM model, only the implementation aspects of the JC model are described here, while the detailed parameter identification procedure is presented later in the calibration section. Initial JC parameters were adopted from Rami et al. (Rami & Kallel et al. 2017), who validated the model for turning operations and residual stress predictions in AISI 4140. These values were used as a starting point because they reproduce the correct order of magnitude of the flow stress for this steel. However, since machining response is highly sensitive to the exact shape of the flow stress surface at high strain rates and temperatures, the parameters were subsequently recalibrated in this work using force measurements and DIC-derived strain and

strain-rate fields. The numerical values of the JC parameters are not fixed at this stage but are identified later through a multistage calibration strategy.

Temperature-dependent material properties

To ensure physically realistic thermomechanical coupling, all relevant workpiece properties were defined as functions of temperature, including thermal conductivity, specific heat capacity, density, Young's modulus and Poisson's ratio. These temperature dependencies (Table 4.3) are essential for correctly predicting plastic dissipation, thermal diffusion, and heat partitioning between chip, tool and workpiece.

Table 4.3: Temperature-dependent physical and mechanical properties of AISI 4140 (Gerstenmeyer 2018).

T (°C)	k (W/m·K)	c_p (J/kg·K)	ρ (kg/m³)	E (GPa)	ν
20	45	460	7850	210	0.30
100	44	500	7830	200	0.30
200	43	540	7800	190	0.30
300	42	560	7780	175	0.295
400	41	590	7750	160	0.290
500	40	620	7720	145	0.285
600	39	640	7700	130	0.280
700	38	660	7680	115	0.275
800	37	680	7650	100	0.270
900	36	700	7620	85	0.265

Tool and coating properties

The thermal properties of the WC–Co substrate and the Al₂O₃ coating were treated as constant, since their temperature dependence in the relevant range is relatively minor compared to steels. The values listed in Table 4.4 were determined experimentally and provide a stable representation of the heat sink behaviour of the tool.

Table 4.4: Constant thermal properties of tool and coating materials

Material	k (W/m·K)	c_p (J/kg·K)	ρ (kg/m³)
WC–Co	85	300	14500
Al ₂ O ₃ coating	3	1000	3900

4.6.4 Decoupled Microstructure Evolution Modelling

Grain refinement during machining results from severe plastic deformation and the associated thermomechanical loading of the material. Under the high strain rates and elevated temper-

atures present in the chip formation zone, dynamic recrystallisation (DRX) can become a dominant mechanism, particularly in the subsurface region.

To model DRX-driven grain evolution, three formulations were implemented and evaluated in this study: (i) an empirical Zener–Hollomon (ZH) model, (ii) a thermodynamic model based on Helmholtz free energy, and (iii) a mechanistic dislocation-density (DD) based model.

The simulation strategy follows a decoupled approach: DRX predictions are computed in post-processing, using as input the strain, strain-rate and temperature fields derived from FEM simulations with the Johnson–Cook material model. In other words, the DRX models do not affect the mechanical solution and no feedback is introduced to remeshing, element deletion or the constitutive behaviour.

This modular strategy enables a direct comparison of DRX models under identical thermomechanical conditions and allows the microstructural analysis to be refined (and recalibrated) without re-running the cutting simulations.

Zener–Hollomon Model

The Zener–Hollomon model is an empirical approach that characterises the combined influence of strain rate and temperature on grain size evolution during high-temperature deformation processes (Zener & Hollomon 1944). It is formulated using the temperature-compensated strain-rate parameter Z , defined as:

$$Z = \dot{\bar{\epsilon}}_{pl} \cdot \exp\left(\frac{Q}{RT}\right), \quad 4.11$$

where $\dot{\bar{\epsilon}}_{pl}$ is the equivalent plastic strain rate, $Q = 116,700$ J/mol is the activation energy for deformation, $R = 8.3145$ J/(mol·K) is the universal gas constant and T is the absolute temperature.

The equivalent plastic strain $\bar{\epsilon}_{pl}$ is a scalar measure of accumulated plastic deformation, obtained from the plastic strain tensor:

$$\bar{\epsilon}_{pl} = \sqrt{\frac{2}{3} \epsilon_{ij}^{pl} \epsilon_{ij}^{pl}}, \quad 4.12$$

and is used here as the internal variable driving DRX.

The dynamically recrystallised grain size d_{DRX} is related to Z by a power law:

$$d_{\text{DRX}} = K_1 \cdot Z^{K_2}, \quad 4.13$$

where K_1 and K_2 are empirically determined material constants (Sellars & Tegart 1966). DRX kinetics are described using the model proposed by Ambrosy and Zanger et al. (Ambrosy & Zanger et al. 2015).

Material constants K_3 to K_9 were adopted from the same source and refined using experimental grain size data, which also defined the initial grain size d_0 .

The recrystallised volume fraction $X^{D(0 \rightarrow 1)} \in [0, 1]$ evolves as a function of plastic strain:

$$X^{D(0 \rightarrow 1)} = 1 - \exp \left[-G \cdot (\bar{\varepsilon}_{pl} - \varepsilon_{cr})^{K_3} \right] \quad 4.14$$

The critical strain is denoted by ε_{cr} , while G is the Avrami-type growth rate coefficient:

$$G = K_4 \cdot (\varepsilon_{0.5}^{K_3})^{-1} \quad 4.15$$

The characteristic strain $\varepsilon_{0.5}$, at which 50% recrystallisation is achieved, is defined by:

$$\varepsilon_{0.5} = K_5 \cdot (K_6 \cdot d_0^{0.5} \cdot Z^{K_7} - \varepsilon_{cr}) \quad 4.16$$

The critical strain itself is modelled as a function of initial grain size and Zener parameter:

$$\varepsilon_{cr} = K_8 \cdot d_0^5 \cdot Z^{K_9} \quad 4.17$$

The grain size at time step $t+1$ is computed as a mixture of recrystallised and unrecrystallised fractions:

$$d_{t+1} = X^{D(0 \rightarrow 1)} \cdot d_{\text{DRX}} + (1 - X^{D(0 \rightarrow 1)}) \cdot d_{0t} \quad 4.18$$

This formulation reflects the gradual transformation of the initial microstructure into dynamically recrystallised grains. As $\bar{\varepsilon}_{pl} > \varepsilon_{cr}$, the recrystallised volume fraction increases sigmoidally, driving grain refinement toward a stable size d_k .

The rate of recrystallisation is given by the following differential form:

$$\dot{X}^{D(0 \rightarrow 1)} = \dot{\bar{\varepsilon}}_{pl} \cdot G \cdot K_3 \cdot (\bar{\varepsilon}_{pl} - \varepsilon_{cr})^{K_3-1} \cdot \exp \left[-G \cdot (\bar{\varepsilon}_{pl} - \varepsilon_{cr})^{K_3} \right] \quad 4.19$$

Table 4.5: Material constants used in the Zener–Hollomon DRX model (adapted from (Sellars & Tegart 1966) and (Ambrosy & Zanger et al. 2015))

Parameter	Description	Value
d_0 [μm]	Initial grain size	5
Q [kJ/mol]	Activation energy for deformation	116.7
R [J/(mol·K)]	Universal gas constant	8.314
K_1 [μm]	Grain size coefficient	2000
K_2 [–]	Grain size exponent (Z-dependence)	0.175
K_3 [–]	Avrami exponent	1.5
K_4 [–]	Growth rate scaling factor	0.7
K_5 [–]	Scaling factor for $\varepsilon_{0.5}$	0.01
K_6 [–]	Grain size scaling in $\varepsilon_{0.5}$	0.005
K_7 [–]	Z-dependence in $\varepsilon_{0.5}$	0.15
K_8 [–]	Scaling factor for ε_{cr}	0.0015
K_9 [–]	Z-dependence in ε_{cr}	0.085

Helmholtz Free Energy Model

The thermodynamic model based on Helmholtz free energy conceptualises dynamic recrystallisation (DRX) as an irreversible, non-isothermal transformation governed by the internal energy and entropy changes within the material. This approach was originally proposed by Poliak and Jonas (Poliak & Jonas 1996) and further developed and applied to machining simulations by Buchkremer et al. (Buchkremer & Klocke et al. 2016).

DRX is treated as a dissipative thermodynamic transition involving continuous evolution in von Mises strain, equivalent strain rate, temperature, and grain size. The fundamental driving quantity is the Helmholtz free energy f , which is defined as:

$$df = du - s \cdot dT - T \cdot ds \quad 4.20$$

where du is the differential change in internal energy, s is entropy, and T is the absolute temperature. The internal energy variation du consists of mechanical, thermal, and interface contributions:

$$du = de_{me} + de_{th} + de_a \quad 4.21$$

The mechanical energy contribution de_{me} arises from plastic deformation and is computed as the integral of the yield stress over the equivalent plastic strain:

$$de_{me} = \int_{\varepsilon_t}^{\varepsilon_{t+1}} \sigma(\varepsilon, \dot{\varepsilon}, T) d\varepsilon \quad 4.22$$

Under metal cutting conditions, the yield stress σ is influenced by strain hardening, strain rate sensitivity, and thermal softening, and is described using the Johnson–Cook constitutive model. Substituting this model into the integral leads to the expression:

$$de_{me} = \left(1 + C \cdot \ln \left(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right)\right) \cdot \left(1 - \left(\frac{\bar{T} - T_0}{T_m - T_0}\right)^m\right) \cdot \left(A \cdot (\varepsilon_{t+1} - \varepsilon_t) + \frac{B}{n+1} \cdot (\varepsilon_{t+1}^{n+1} - \varepsilon_t^{n+1})\right) \quad 4.23$$

The final recrystallised grain size d_{t+1} is computed from the mechanical energy dissipation and grain boundary energy considerations as follows:

$$d_{t+1} = \frac{3 \cdot \gamma(T)}{\frac{3 \cdot \gamma(T)}{d_t} + \Omega(T) \cdot \int (1 - \beta) de_{me}} \quad 4.24$$

Here, $\gamma(T)$ represents the specific grain boundary energy as a function of temperature, and $\Omega(T)$ denotes the fraction of mechanical energy stored in the material in the form of dislocations.

The parameter β accounts for the recrystallisation growth rate and varies between 0 and 1. The energy conversion efficiency $\Omega(T)$ is given by:

$$\Omega(T) = \omega_1 - \omega_2 \cdot \left(\frac{T}{T_m}\right) \quad 4.25$$

This temperature-dependent formulation reflects the decreasing stored energy as dynamic recovery dominates at elevated temperatures.

The onset of recrystallisation is controlled by the material's melting temperature T_m , and the grain boundary energy factor $\gamma(T)$ is derived using the empirical relationship:

$$\gamma(T) = a + b \cdot T \quad 4.26$$

where a and b are empirically fitted constants. The model constants were obtained from the literature (Buchkremer & Klocke et al. 2016) and refined during simulation calibration.

Table 4.6: Helmholtz Free Energy Model Parameters (adapted from (Buchkremer & Klocke et al. 2016))

Parameter	Description	Value
<i>Initial Conditions and General Constants</i>		
d_0 [μm]	Initial grain size	5
T_m [K]	Melting temperature	1809
T_0 [K]	Reference temperature	293
β [–]	recrystallisation efficiency	0.9
<i>Grain Boundary Energy</i>		
a [J/m^2]	Grain boundary energy offset	4.9×10^{-10}
b [$\text{J}/(\text{m}^2 \cdot \text{K})$]	Temperature coefficient of grain boundary energy	4.2×10^{-6}
<i>Stored Energy Conversion</i>		
ω_1 [–]	Scaling parameter	1.667
ω_2 [–]	Temperature scaling	0.667

Dislocation Density Model

Microstructural refinement during machining is described using a dislocation-density-based model originally developed by Estrin and Kim (Estrin & Kim 2007). The formulation resolves the evolution of deformation-induced substructure and provides a physically motivated prediction of grain refinement without explicitly tracking crystallographic orientations or misorientations. The material is subdivided into *cell interiors* and *cell walls*, characterised by distinct dislocation densities ρ_c and ρ_w , respectively. Grain refinement emerges from the competition between dislocation accumulation, transfer between substructural domains, and dynamic recovery.

Assuming that both substructural regions deform at the same shear rate, the equivalent shear rate $\dot{\gamma}_r$ is related to the macroscopic strain rate $\dot{\varepsilon}$ through the Taylor factor M_T :

$$\dot{\gamma}_r = M_T \dot{\varepsilon} = \dot{\gamma}_c^r = \dot{\gamma}_w^r. \quad 4.27$$

The evolving substructure is characterised by the cell-wall volume fraction f_w , which transitions from an initial value f_0 toward a stable asymptotic value f_∞ with increasing cumulative shear strain γ_r , reflecting progressive subdivision of the dislocation structure:

$$f_w = f_\infty + (f_0 - f_\infty) \exp\left(-\frac{\gamma_r}{\tilde{\gamma}_r}\right). \quad 4.28$$

The evolution of dislocation densities in the cell interiors and cell walls is governed by dislocation multiplication, transfer between domains, and annihilation through dynamic recovery. For

the cell interiors,

$$\dot{\rho}_c = \alpha^* \frac{1}{\sqrt{3}b} \sqrt{\rho_w} \dot{\gamma}_r - \beta^* \frac{6}{b d_{dd} (1 - f_w)^{1/3}} \dot{\gamma}_r - k_0 \left(\frac{\dot{\gamma}_r}{\dot{\gamma}_0} \right)^{-1/n_{dd}} \rho_c \dot{\gamma}_r, \quad 4.29$$

and for the cell walls,

$$\dot{\rho}_w = \beta^* \sqrt{\frac{3}{1 - f_w}} \frac{1}{b} \sqrt{\rho_w} \dot{\gamma}_r + \beta^* \frac{6}{b d_{dd}} (1 - f_w)^{2/3} \left(\frac{\dot{\gamma}_r}{\dot{\gamma}_0} \right)^{1/4} \rho_w^{7/6} - k_0 \left(\frac{\dot{\gamma}_r}{\dot{\gamma}_0} \right)^{1/4} \rho_w^2. \quad 4.30$$

The instantaneous total dislocation density predicted by the substructure model is obtained via a rule of mixtures:

$$\dot{\rho}_{\text{tot}} = f_w \rho_w + (1 - f_w) \rho_c. \quad 4.31$$

The characteristic grain size resulting from deformation-induced refinement is derived directly from the total dislocation density using the established inverse square-root relationship (Estrin & Tóth et al. 1998):

$$d_f = \frac{K_{dd}}{\sqrt{\dot{\rho}_{\text{tot}}}}. \quad 4.32$$

The grain size d_f represents the primary microstructural output of the dislocation-density model and is used for direct comparison with experimentally measured subsurface grain-size profiles.

Although the model directly predicts grain size, comparable levels of refinement may arise from distinct physical mechanisms. To distinguish between refinement dominated by severe plastic deformation and that associated with thermally activated dynamic recrystallisation, an interpreted recrystallised fraction X_{DRX} is introduced as a diagnostic quantity.

The initial dislocation density ρ_0 , measured prior to machining (e.g. by X-ray diffraction), is taken as representative of a recovered, low-dislocation-density state. Assuming that newly recrystallised grains rapidly recover toward a comparable state, the effective dislocation density after partial DRX is expressed as

$$\rho_{\text{tot}} = (1 - X_{\text{DRX}}) \dot{\rho}_{\text{tot}} + X_{\text{DRX}} \rho_0. \quad 4.33$$

Solving for X_{DRX} yields

$$X_{\text{DRX}} = \frac{\dot{\rho}_{\text{tot}} - \rho_{\text{tot}}}{\dot{\rho}_{\text{tot}} - \rho_0}, \quad X_{\text{DRX}} \in [0, 1]. \quad 4.34$$

A threshold value X_0 is employed to identify regions where grain refinement is significantly influenced by DRX. Regions with $X_{\text{DRX}} < X_0$ are interpreted as mechanically dominated, whereas regions with $X_{\text{DRX}} \geq X_0$ are classified as DRX-affected.

It is emphasised that grain size alone is insufficient to identify the underlying refinement mechanism. Mechanically refined layers are characterised by elevated dislocation density and stored energy, which may be detrimental to certain mechanical properties. In contrast, DRX-dominated refinement corresponds to a dislocation-poor microstructure that is commonly associated with enhanced microstructural stability.

4.6.5 Calibration of the FEM and Dislocation-Density DRX Model

Among the three DRX formulations evaluated in this work the calibration procedure is developed exclusively for the DD model because it is the only framework that explicitly links the evolving microstructure to the local strain, strain-rate and temperature histories provided by the FEM. Unlike the ZH and Helmholtz approaches, which rely on empirical activation laws or phenomenological driving potentials, the DD formulation resolves the underlying dislocation storage, transfer and recovery mechanisms that govern grain refinement in machining.

Consequently, a dedicated multistage calibration strategy is implemented for the DD model to ensure a physically consistent prediction of subsurface grain size and DRX depth across all cutting conditions. The numerical framework employs a sequential three-stage calibration strategy to ensure that the thermomechanical fields provided to the dislocation-density DRX model are consistent with the experimentally observed mechanical and thermal conditions.

Because the DRX formulation is applied in a decoupled manner, receiving strain, strain-rate and temperature histories from the FEM solution without altering the mechanical response, the upstream FEM calibration must be physically accurate before any microstructural parameter identification is performed. Figure 4.23 summarises the complete three-loop calibration workflow that couples mechanical, thermal, and microstructural identification stages:

- (i) mechanical calibration of the Johnson–Cook (JC) constitutive parameters using dynamometer forces and DIC-derived shear strain and shear-rate paths in the primary deformation zone (PDZ);
- (ii) thermal calibration of the tool–chip–workpiece interface properties using thin-film sensor and thermocouple temperature measurements;
- (iii) microstructural calibration of the DD model parameters using FIB/SEM grain-size profiles, DRX depth and XRD-measured initial dislocation density.

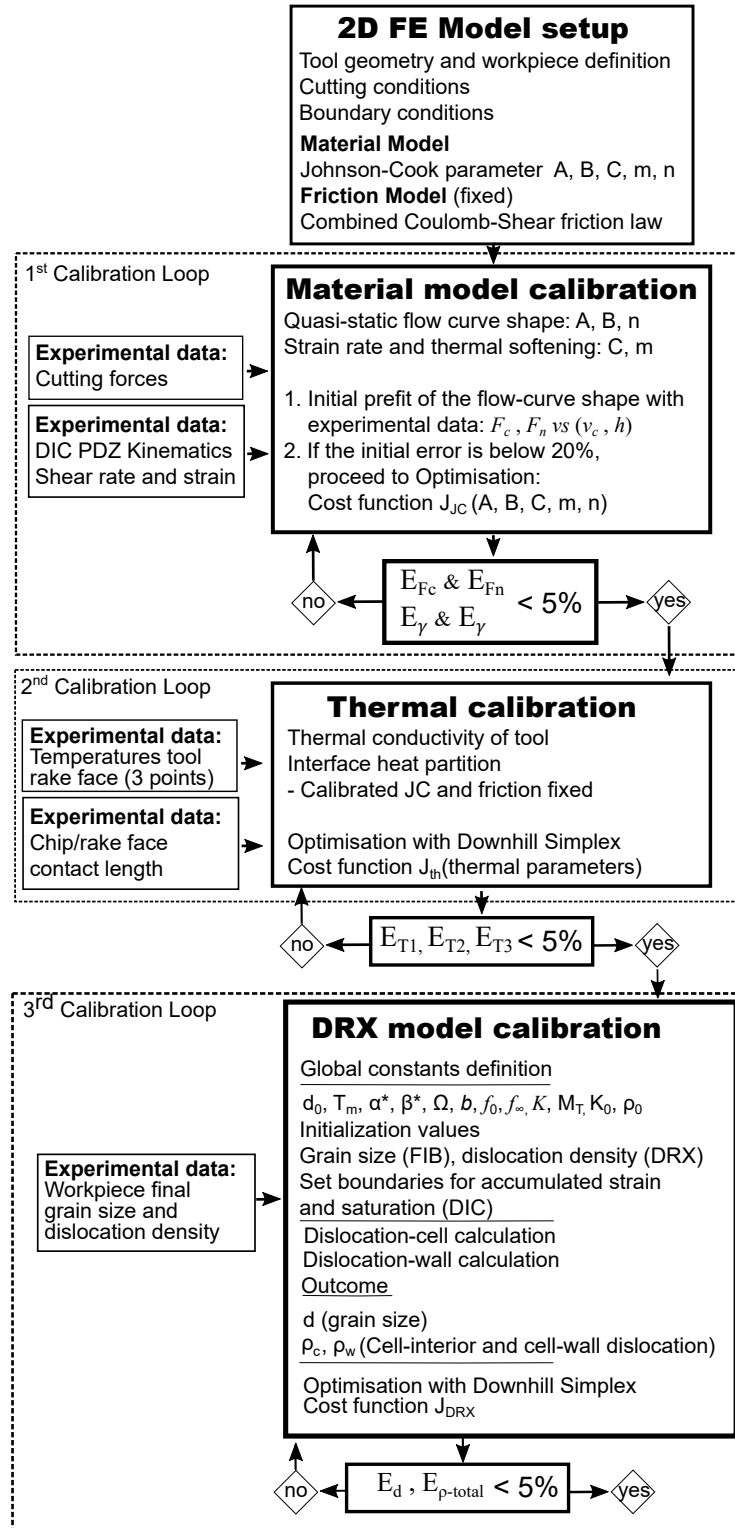


Figure 4.23: Simulation workflow for DRX modelling. The procedure integrates Johnson–Cook calibration, thermal field matching, and post-processing using three decoupled DRX models to predict subsurface grain evolution.

Loop 1: Calibration of the Johnson–Cook Constitutive Parameters

The first calibration loop identifies the Johnson–Cook parameters (A, B, C, n, m) that govern the material flow stress. This stage ensures that the FEM model reproduces both the global cutting forces and the local deformation kinematics in the PDZ. The calibration relies on several experimentally measured quantities. The cutting and passive forces recorded with the three-component dynamometer for each (v_c, h) combination provide the global mechanical response against which the simulated forces are matched. Local deformation kinematics are obtained from high-speed DIC, from which the shear strain histories $\gamma_r^{\text{DIC}}(s)$ and the corresponding shear-rate histories $\dot{\gamma}_r^{\text{DIC}}(s)$ are extracted along streamlines traversing the primary deformation zone. These kinematic fields serve as direct constraints for the strain-hardening, strain-rate sensitivity and thermal-softening components of the Johnson–Cook model. No temperature data are used at this stage, as thermal quantities are introduced exclusively in Loop 2 during the calibration of interfacial heat transfer and thermal boundary conditions.

Initial JC parameters were taken from Rami et al. (Rami & Kallel et al. 2017), supplemented with temperature-dependent elastic and thermal properties from Gerstenmeyer (Gerstenmeyer 2018). These values establish the baseline mechanical response before optimisation. The identification of the Johnson–Cook parameters (A, B, C, n, m) is formulated as a nonlinear least-squares problem. The objective function combines global force response and local deformation kinematics, ensuring that the calibrated material law simultaneously reproduces the measured cutting forces and the DIC-derived strain and strain-rate histories in the primary deformation zone. The cost function is defined as:

$$\begin{aligned}
 J_{\text{JC}} = & w_F \sum_i \left(F_i^{\text{FEM}} - F_i^{\text{exp}} \right)^2 \\
 & + w_\gamma \sum_i \int \left[\gamma_r^{\text{FEM}}(s) - \gamma_r^{\text{DIC}}(s) \right]^2 ds \\
 & + w_{\dot{\gamma}} \sum_i \int \left[\dot{\gamma}_r^{\text{FEM}}(s) - \dot{\gamma}_r^{\text{DIC}}(s) \right]^2 ds.
 \end{aligned} \tag{4.35}$$

Here, F_i^{exp} are the dynamometer-measured cutting and passive forces, while $\gamma_r^{\text{DIC}}(s)$ and $\dot{\gamma}_r^{\text{DIC}}(s)$ denote the experimentally observed shear strain and shear-rate histories extracted from high-speed DIC along PDZ streamlines. The force residuals predominantly constrain the quasi-static hardening parameters (A, B, n) , whereas the DIC-based strain and strain-rate residuals provide critical sensitivity to the strain-rate coefficient C and the thermal-softening exponent m .

This calibration procedure builds on the collaborative optimisation framework established with Stampfer et al. (Stampfer & González et al. 2021b), where automated input generation and simulation control were implemented for material model integration in *Simufact Forming*.

In contrast to earlier approaches such as Agmell et al. (Agmell & Ahadi et al. 2011), which relied solely on force matching, the present method incorporates DIC-based shear strain and shear-rate histories as direct constraints of the internal deformation field. This enables a substantially more accurate identification of strain-rate and temperature sensitivity, which are essential for machining simulations.

A Downhill Simplex algorithm is employed to minimise J_{JC} . Convergence is achieved when the deviations in force, cumulative shear strain and shear rate fall below 5%. The resulting parameter set (Table 4.7) shows a normalised deviation of only 3.1%, indicating excellent agreement between experiment and simulation.

Table 4.7: Optimised Johnson–Cook parameters for AISI 4140 (this work).

A (MPa)	B (MPa)	C	m	n	δF_n (%)
619	659	0.0223	0.9741	0.1219	3.1

Loop 2: Calibration of Thermal Boundary Conditions

The second calibration loop determines the thermal boundary parameters governing heat flow at the tool–chip–workpiece interfaces. Here only thermal experimental data are used. The temperature distribution measured on the rake face using thin-film thermocouple sensors provides the primary constraint for calibrating the heat transfer behaviour at the tool–chip interface. Additional temperature measurements taken inside the tool or workpiece by embedded thermocouples complement this dataset and allow the thermal gradients and heat flow paths to be accurately reconstructed. During this loop the mechanical field—namely the strain, strain rate and flow stress histories obtained from Loop 1—remains fixed and is not altered. Likewise, the friction parameters are kept constant throughout all stages of calibration to ensure consistency between mechanical and thermal simulations.

The initial temperature-dependent conductivity and heat capacity of AISI 4140 are taken from Gerstenmeyer (Gerstenmeyer 2018), and the tool–coating properties from in-house measurements (Table 4.4). Heat partition ratio is initially assumed based on classical Oxley values. To identify the thermal boundary parameters governing heat flow at the tool–chip interface, the following thermal cost function is formulated to quantify the deviation between simulated and measured temperatures:

$$J_{\text{th}} = w_T \sum_i \left[T^{\text{FEM}}(x_i) - T^{\text{exp}}(x_i) \right]^2. \quad 4.36$$

Convergence is reached when the deviation between simulated and measured temperatures falls below 5%, yielding a fully validated thermomechanical history $\{\gamma_r(s), \dot{\gamma}_r(s), T(s)\}$ for microstructural modelling.

Loop 3: Calibration of the Dislocation-Density DRX Model

The final calibration loop identifies the parameters of the dislocation-density DRX model using the validated FEM deformation histories together with the experimentally observed subsurface microstructure. The experimental inputs required at this stage comprise the FIB/SEM grain-size profiles $d_f^{\text{exp}}(z)$ for each (v_c, h) combination, as well as the measured DRX depth, defined as the depth where the grain size falls below $1 \mu\text{m}$.

The initial dislocation density ρ_0 is taken from XRD measurements prior to machining and provides the starting stored-energy level for the DD evolution equations. In addition, the temperature histories $T(s)$ along the FEM streamlines, together with the shear-strain $\gamma_r(s)$ and shear-rate $\dot{\gamma}_r(s)$ histories, obtained from the thermomechanically validated simulation of Loops 1 and 2 and already cross-validated against the DIC measurements, serve as the driving fields for the microstructural integration.

The DD model parameters are initialised using literature values for BCC steels, primarily following Estrin (Estrin & Kim 2007) and Ding (Ding & Shin 2014). This provides starting estimates for the dislocation generation coefficient α^* , the transfer coefficient β^* , and the annihilation factor k_0 , as well as for the geometric parameters f_0 , f_∞ , and the reference shear strain $\tilde{\gamma}_r$. The grain-size scaling factor K_{dd} is also initialised from literature. The experimentally measured initial grain size $d_0 = 5 \mu\text{m}$ is used to initialise the grain-size state, and the initial dislocation density ρ_0 is fixed from the XRD measurements before cutting. These inputs define the baseline microstructural state from which the DD evolution is integrated along the FEM strain–rate–temperature paths during optimisation.

To identify the model parameters θ that govern dislocation multiplication, transfer, recovery, and geometric evolution of the cell structure, a two-part cost function is minimised:

$$J_{\text{DRX}} = J_{\text{grain}} + J_{\text{DRX-depth}}, \quad 4.37$$

where J_{grain} enforces agreement with the full subsurface grain-size profiles and $J_{\text{DRX-depth}}$ constrains the experimentally observed depth of the recrystallised layer. The grain-size mismatch term is defined as:

$$J_{\text{grain}} = w_d \sum_{i,z} \left[d_{f,i}^{\text{model}}(z; \theta) - d_{f,i}^{\text{exp}}(z) \right]^2, \quad 4.38$$

where $d_{f,i}^{\text{exp}}(z)$ are the FIB-measured grain sizes at various depths z and for various cutting conditions (v_c^i, h^i) . This term calibrates the overall curvature and magnitude of grain refinement predicted by the model. In particular, it constrains the balance between dislocation multiplication (α^*), transfer (β^*), and annihilation (k_0), as well as the scaling factor K_{dd} that translates dislocation density to grain size. The second term enforces agreement with the measured DRX depth:

$$J_{\text{DRX-depth}} = w_Z \sum_i \left[Z_{d < 1\mu\text{m}}^{\text{model}}(v_c^i, h^i; \theta) - Z_{d < 1\mu\text{m}}^{\text{exp}}(v_c^i, h^i) \right]^2. \quad 4.39$$

Here, $Z_{d < 1\mu\text{m}}^{\text{exp}}$ is the depth at which FIB/SEM measurements show grain sizes below $1\mu\text{m}$. This term is particularly sensitive to the critical strain for DRX onset, to the evolution of the wall fraction $f_w(z)$, and to recovery parameters that regulate saturation of dislocation density at high temperature. A Downhill Simplex algorithm minimises J_{DRX} . For each trial parameter set, the DD evolution equations are integrated along the validated FEM streamline histories. Because the thermomechanical fields are fixed from Loops 1 and 2, Loop 3 yields a unique and physically consistent parameter set.

Table 4.8: Final calibrated parameters of the dislocation-density DRX model.

Parameter	Description	Calibrated value
d_0 [μm]	Initial grain size	5
ρ_0 [m^{-2}]	Initial dislocation density (XRD)	9.00×10^{14}
f_0 [–]	Initial cell wall fraction	0.25
f_∞ [–]	Minimum cell wall fraction	0.05
$\tilde{\gamma}_r$ [–]	Reference shear strain	4.0
T_m [K]	Melting temperature	1809
b [m]	Burgers vector	2.48×10^{-10}
M_T [–]	Taylor factor	2.8
α^* [–]	Dislocation generation coefficient	6.00×10^{-5}
β^* [–]	Dislocation transfer coefficient	1.20×10^{-6}
k_0 [–]	Dislocation annihilation factor	1.17×10^{-5}
K_{dd} [m^{-1}]	Grain size scaling factor	4.26×10^7

4.6.6 3D Chip Formation Modelling

Three-dimensional finite element simulations were performed to extend the calibrated 2D thermomechanical and microstructural framework to realistic turning conditions. Compared to the plane-strain formulation, the 3D model captures out-of-plane chip flow, spatially varying tool engagement along the cutting edge, and wear-induced changes in contact mechanics that cannot be reproduced in two dimensions.

The workpiece was discretised using structured hexahedral elements with a minimum edge length of $1\ \mu\text{m}$ in the near-surface region, and adaptive remeshing was employed to refine zones exhibiting steep gradients in strain, strain rate, or temperature.

A two-phase, multi-pass cutting strategy was adopted, consistent with the quasi-steady-state method established in the 2D framework. The first phase models the interaction of a pristine cutting edge with an undeformed surface, producing the baseline thermomechanical fields of the virgin material. In the second phase, the tool cuts through a surface layer previously modified by the first pass.

The temperature field, plastic strain history, stress components, and the grain size predicted by the DD model are transferred between passes, allowing the cumulative thermomechanical and microstructural evolution to be represented accurately. This iterative mapping procedure reflects the physical history of the workpiece and enables realistic prediction of multi-pass surface integrity.

Figure 4.24 summarises the 3D configuration. Subfigure (a) shows the full turning model, where the tool is treated as an ideally rigid, heat-conductive body. Subfigure (b) highlights the local tool–workpiece interaction during external longitudinal turning. Subfigure (c) illustrates the two-step multi-pass strategy used to accumulate thermomechanical load effects.

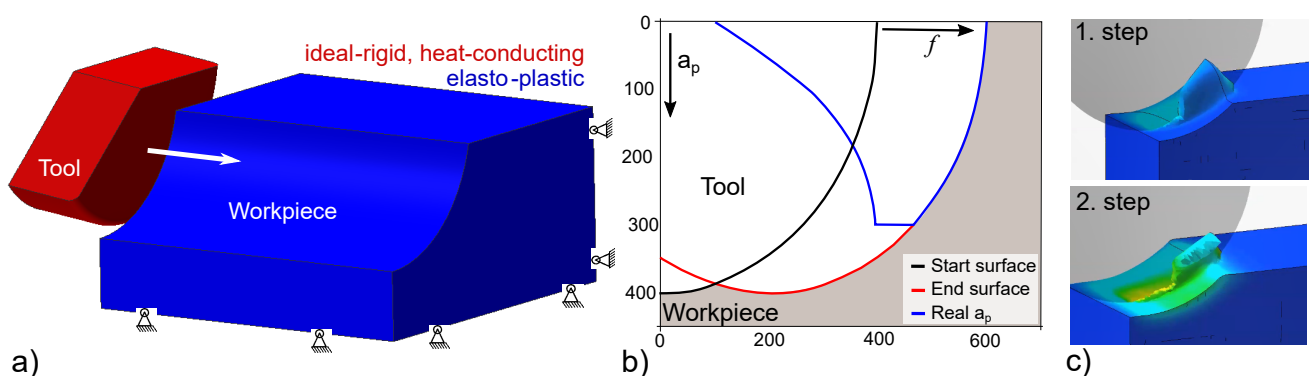


Figure 4.24: Setup for 3D machining simulations: (a) Full 3D turning model; (b) Local geometric conditions during external longitudinal turning; (c) Multi-pass simulation sequence for capturing cumulative effects on surface integrity.

Extension of the Dislocation-Density Model to 3D

The dislocation-density (DD) model formulated in Section 4.6.4 relies on scalar driving variables (accumulated shear strain, shear rate, temperature). In 3D FEM, plastic deformation is tensorial, and thus an equivalent shear rate must be derived from the plastic strain-rate tensor $\dot{\varepsilon}_{ij}^{pl}$. The equivalent shear rate is obtained from the second invariant of the deviatoric plastic strain-rate tensor:

$$\dot{\gamma}_r = M_T \cdot \sqrt{\frac{2}{3} \dot{\varepsilon}_{ij}^{pl} \dot{\varepsilon}_{ij}^{pl}}, \quad 4.40$$

using the Taylor factor M_T . This definition preserves the scalar structure of the DD formulation while incorporating the multiaxial loading state inherent to 3D chip formation. Based on this tensor-derived shear rate, the evolution of cell-interior and cell-wall dislocation densities becomes:

$$\dot{\rho}_c = \alpha^* \frac{1}{\sqrt{3}b} \sqrt{\rho_w} \dot{\gamma}_r - \beta^* \frac{6}{b d_{dd} (1 - f_w)^{1/3}} \dot{\gamma}_r - k_0 \left(\frac{\dot{\gamma}_r}{\dot{\gamma}_0} \right)^{-1/n_{dd}} \rho_c \dot{\gamma}_r, \quad 4.41$$

$$\dot{\rho}_w = \beta^* \sqrt{\frac{3}{1 - f_w} \frac{\rho_w}{b}} \dot{\gamma}_r + \beta^* \frac{6}{b d_{dd}} (1 - f_w)^{2/3} \left(\frac{\dot{\gamma}_r}{\dot{\gamma}_0} \right)^{1/4} \rho_w^{7/6} - k_0 \left(\frac{\dot{\gamma}_r}{\dot{\gamma}_0} \right)^{1/4} \rho_w^2. \quad 4.42$$

The total dislocation density and resulting grain size follow the same expressions as in the 2D model:

$$\rho_{\text{tot}} = f_w \rho_w + (1 - f_w) \rho_c, \quad d = \frac{K_{dd}}{\sqrt{\rho_{\text{tot}}}}. \quad 4.43$$

This reformulation enables direct application of the calibrated DD model within 3D cutting simulations while retaining the physical interpretation of the dislocation storage, transfer, and recovery mechanisms.

Tool Wear Modelling in 3D FEM

Wear-induced changes in the tool geometry were incorporated parametrically to evaluate their influence on contact mechanics, thermal loading, and microstructural evolution. Idealised representations of adhesive wear, abrasive wear, and edge rounding were generated (Figure 4.25) and introduced directly as static tool geometries. Seven discrete wear levels were simulated: $VB = 0, 50, 100, 150, 200, 250$, and $300 \mu\text{m}$. After each simulation, the

temperature field, stress state, and plastic strain field were exported and mapped onto the updated geometry for the next wear increment.

To ensure thermal continuity, the volumetric temperature field of the tool was preserved and remapped between simulations, allowing cumulative heat effects to be represented accurately across successive wear states. This procedure produced a comprehensive database of 3D thermomechanical and microstructural outcomes across the full factorial design of cutting parameters and wear levels. These results form the basis for the regression-based surrogate models and the Bayesian wear-inference framework developed in the subsequent chapters.

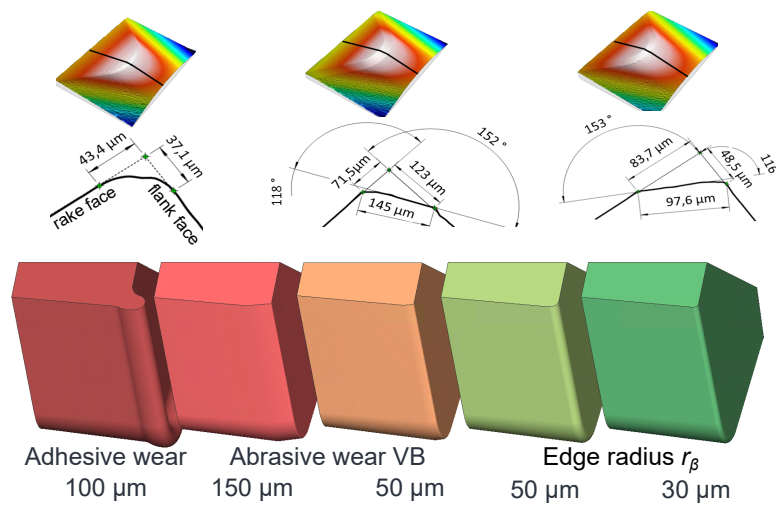


Figure 4.25: Tool wear integration in 3D FE simulations, showing idealised representations of adhesive wear, abrasive wear, and edge rounding.

4.7 Bayesian Inference for Tool Wear Prediction

The integration of three-dimensional FEM simulations with regression-based surrogate models provides a physically grounded basis for predicting microstructural responses such as subsurface grain refinement. However, the predictive quality of these models depends critically on the availability of accurate information on the current tool-wear state. Since flank wear VB cannot be measured continuously during machining and is typically obtained only at discrete inspection intervals, its evolution must be inferred under uncertainty.

To address this limitation, a Bayesian inference framework is introduced to estimate the current wear state using limited observations, process knowledge, and physically motivated prior distributions. It is important to emphasise that Bayesian inference is applied exclusively to the estimation of tool wear. Microstructural outputs (grain size, recrystallised depth, DRX fraction) remain deterministic predictions obtained either directly from the calibrated 3D FEM simulations or from surrogate models trained on the FEM database. The Bayesian model

therefore acts as a probabilistic *selector* that identifies which simulated wear geometry, and thus which microstructural prediction, is most plausible at a given cutting time.

4.7.1 Bayesian Wear Rate Model

Flank wear progression is represented using the classical exponential growth model,

$$VB(t) = b \exp(at), \quad 4.44$$

where a is the wear growth rate and b the initial wear level, capturing microscopic pre-existing defects or early adhesive wear. This model form is consistent with the experimentally observed evolution of flank wear under the tested turning conditions.

Weakly informative priors are assigned to the unknown parameters,

$$a \sim \mathcal{U}(0, 0.2), \quad b \sim \mathcal{U}(0, 0.2),$$

covering the physically plausible parameter range. Measurement uncertainty is captured using a half-normal prior,

$$\sigma_{VB} \sim \text{Half-Normal}(0, 0.1),$$

ensuring positivity and concentrating mass on small but non-negligible noise levels.

4.7.2 Likelihood and Posterior Formulation

For a wear measurement VB_i obtained at cutting time t_i , the observation model is

$$p(VB_i \mid a, b, \sigma_{VB}) = \mathcal{N}(VB_i \mid b \exp(at_i), \sigma_{VB}^2), \quad 4.45$$

where the Gaussian noise term represents uncertainty in the flank-wear observations and residual discrepancy of the exponential wear model.

Given n observations, the posterior distribution for (a, b, σ_{VB}) follows from Bayes' rule:

$$p(a, b, \sigma_{VB} \mid VB_{1:n}) \propto p(a) p(b) p(\sigma_{VB}) \prod_{i=1}^n p(VB_i \mid a, b, \sigma_{VB}). \quad 4.46$$

Posterior inference is performed using Hamiltonian Monte Carlo with the No-U-Turn Sampler (NUTS). Convergence diagnostics satisfy $\hat{R} < 1.01$, bulk and tail ESS > 400 , and no divergent transitions, ensuring reliable characterisation of the posterior.

4.7.3 Integration With the FEM Simulation Database

Posterior samples of (a, b) generate a family of admissible wear trajectories $VB(t)$. Each sampled wear value corresponds to one of the discrete wear states in the 3D FEM database. When a sampled wear state lies between discretised simulation levels, interpolation is performed using the regression model trained on the full-factorial FEM dataset.

This probabilistic mapping enables uncertainty-aware predictions of subsurface grain size evolution and DRX depth, temperature and stress fields, equivalent plastic strain distributions, and surface integrity metrics derived from the DD-based model. Thus, while the DRX prediction itself is deterministic, the *selection of the relevant FEM state* is probabilistic and governed by the Bayesian inference model. Bayesian inference supplies a probabilistic wear estimate, which determines which FEM or regression-based prediction is most appropriate.

4.7.4 Sequential Updating via Recursive Bayesian Inference

A key advantage of the Bayesian formulation is its ability to incorporate new wear measurements recursively. Let

$$p(a, b, \sigma_{VB} \mid VB^{(t)})$$

denote the posterior distribution after incorporating data up to time t . Upon acquiring a new measurement $VB^{(t+1)}$, the distribution is updated as

$$p(a, b, \sigma_{VB} \mid VB^{(t+1)}) \propto p(a, b, \sigma_{VB} \mid VB^{(t)}) p(VB^{(t+1)} \mid a, b, \sigma_{VB}), \quad 4.47$$

In practice, MCMC sampling is initialised from the previous posterior, which can reduce the computational effort required for sequential re-estimation. This recursive update mechanism provides the methodological basis for process-accompanying monitoring. As new wear measurements become available, the posterior distribution of the wear parameters can be updated and propagated through the regression model, yielding sequentially refined grain-size predictions that reflect the estimated tool state. By coupling probabilistic wear estimation with the high-fidelity FEM database, the framework provides uncertainty-aware predictions of thermomechanical loads and surface integrity evolution, effectively linking data-driven inference with physically based simulation.

4.8 Soft Sensor Architecture

A soft sensor is a virtual sensing framework that reconstructs latent or difficult-to-measure process quantities by combining physics-based modelling with data-driven inference. In the present work, a hybrid soft sensor is developed to predict the evolution of surface integrity during machining by integrating high-fidelity 3D FEM simulations, regression-based surrogate

modelling, and Bayesian inference for tool-wear estimation. The architecture supports offline prediction based on process parameters, material data and tool geometry, as well as sequential refinement when new measurements become available. The system is implemented in an open-loop configuration and is structured as a basis for future on-machine and closed-loop deployment.

4.8.1 Summary of Model Construction and Calibration

The soft sensor builds upon the calibrated modelling chain developed in the previous sections. Orthogonal cutting experiments were conducted to characterise forces, temperatures, deformation kinematics and subsurface microstructures across a controlled range of cutting speeds, tool geometries and wear states. These measurements formed the basis for calibrating the 2D FEM framework, where flow stress, friction behaviour and DRX kinetics were identified using dynamometer forces, thin-film temperature sensing and DIC-derived strain paths.

The calibrated models were subsequently implemented in 3D FEM simulations, which were validated against turning experiments and executed across a full factorial matrix in cutting speed, feed rate and tool-wear increments. Each simulation yielded detailed thermomechanical fields and microstructural outputs, including grain size, recrystallised volume fraction and plastic-strain gradients, which formed a high-fidelity database.

Regression-based surrogate models were then trained on this database to interpolate microstructural responses over the continuous machining parameter space. Once trained, these surrogate models constitute the computational core of the soft sensor, enabling rapid surface integrity prediction without rerunning FEM simulations.

4.8.2 Sequential Updating and Hybrid Integration

A major challenge for surrogate-based prediction in machining is the need for accurate knowledge of the current tool-wear state, which is rarely available in real time. To address this, a Bayesian inference module is introduced to estimate flank wear from cutting time and sparse measurements. Tool wear is modelled using an exponential degradation law whose parameters are inferred via Hamiltonian Monte Carlo sampling. This yields a posterior distribution of the wear trajectory, from which point estimates and credible intervals are obtained.

A key feature of the Bayesian framework is its recursive updating capability. When a new wear observation becomes available, the previous posterior distribution is used as the prior for the subsequent inference step, and the model is re-estimated using the additional observation. The updated wear-state distribution is propagated through the surrogate regression model,

yielding refined predictions of microstructural metrics such as grain size, DRX depth and recrystallised volume fraction.

Notably, Bayesian inference is used exclusively to infer *tool wear*; microstructural quantities are always obtained deterministically from the FEM database and its surrogate interpolation. The overall hybrid architecture operates along two interconnected pathways. The *offline* path comprises experimental characterisation, 2D model calibration, 3D simulation and surrogate-model construction. The *sequential-update* path combines Bayesian wear estimation with the surrogate model to provide updated, uncertainty-aware surface-integrity predictions.

This workflow is illustrated schematically in Fig. 4.26. The diagram highlights the interplay between 2D model calibration, 3D simulations, the FEM database, regression models and Bayesian inference, and shows how tool-wear estimates drive both offline and sequentially updated grain-size predictions.

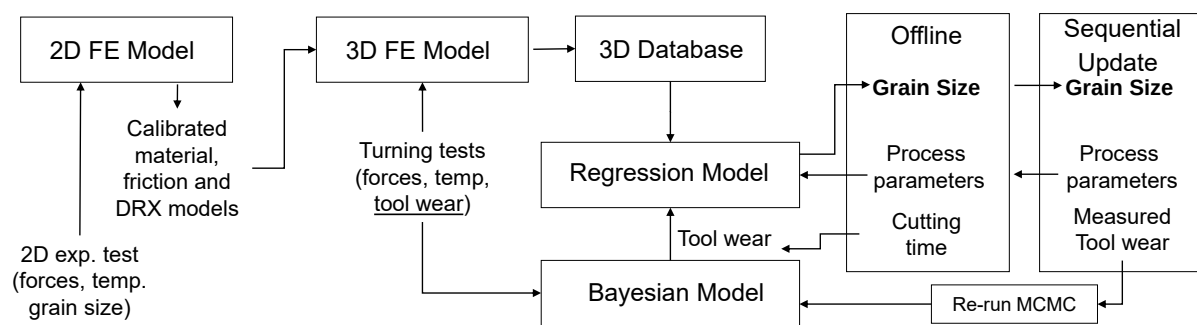


Figure 4.26: Hybrid modelling framework integrating FEM simulations, surrogate regression and Bayesian wear inference for uncertainty-aware surface-integrity prediction.

5 Results of Orthogonal Cutting Processes

This chapter presents the results of orthogonal cutting experiments and simulations, with a central focus on evaluating the surface integrity of the machined workpiece. Key process response variables—including cutting forces, temperature evolution, strain fields, hardness distribution, and grain size—are analysed using both experimental methods and finite element modelling. Finally, the accuracy, applicability, and limitations of the FEM models are assessed through comparison with experimental observations.

5.1 Experimental Results

5.1.1 Force and Temperature Measurements

Cutting forces and temperatures during 2D orthogonal cutting were investigated through linear orthogonal tests using the setup described in Section 4.5.1. The measured results, shown in Figure 5.1, illustrate the influence of cutting speed v_c and uncut chip thickness h on the mechanical and thermal response of the process.

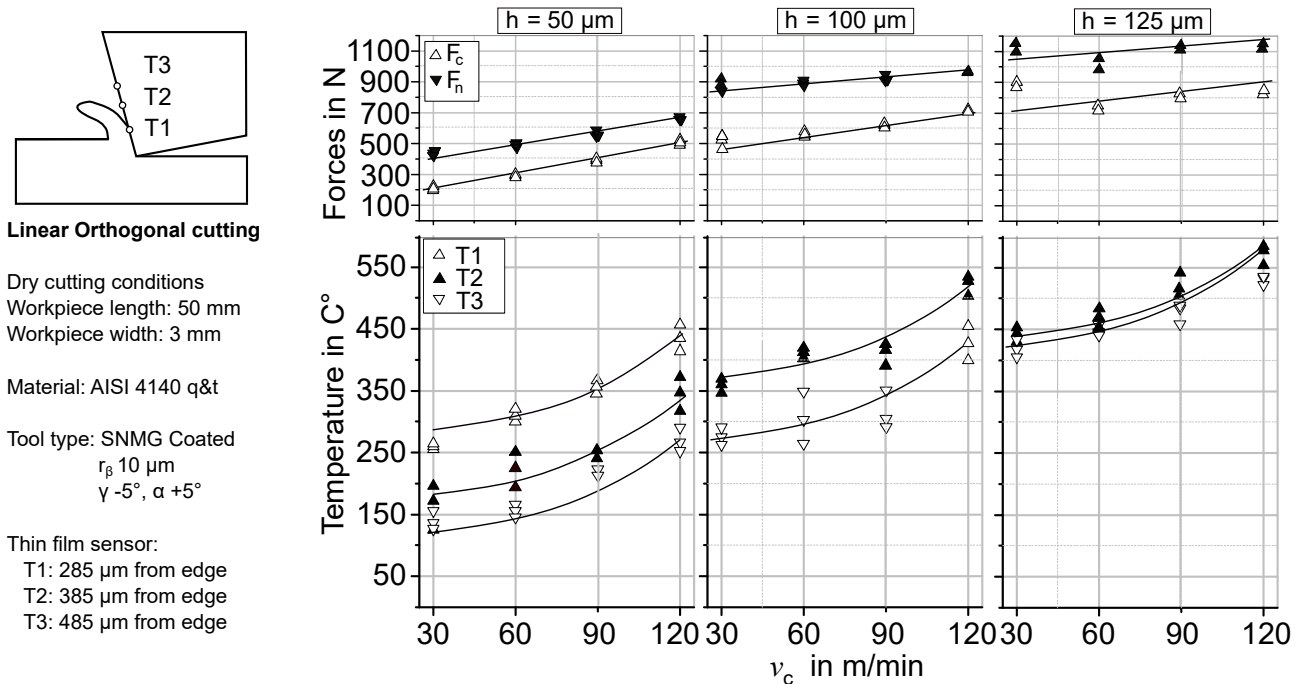


Figure 5.1: Measurements of cutting forces and temperatures for different cutting speeds and chip thicknesses during linear orthogonal cutting process.

For all investigated cutting speeds, both tangential (F_c) and normal (F_n) force components increase monotonically with increasing uncut chip thickness h , reflecting the higher material removal rate and enlarged deformation volume. At lower cutting speeds, an increased scatter of the force signals is observed, particularly at small h , indicating reduced process stability

under dry cutting conditions. Over the investigated range of cutting speeds, no pronounced systematic dependence of force magnitude on v_c can be identified, especially at larger chip thicknesses.

In contrast to the mechanical response, the thermal response exhibits a strong and non-linear dependence on both v_c and h . The measured interface temperatures increase with increasing cutting speed for all chip thicknesses, with higher absolute temperature levels observed at larger h . This trend indicates an enhanced conversion of mechanical work into heat at elevated cutting speeds and chip loads. While linear fits are insufficient to describe the temperature evolution, the measurements consistently show an accelerated temperature rise at higher v_c .

The use of multiple thin-film sensors enables a qualitative assessment of the temperature distribution along the tool rake face. At small uncut chip thicknesses, clear temperature differences between sensors T_1 , T_2 , and T_3 are observed, indicating pronounced spatial gradients along the tool–chip contact region. With increasing uncut chip thickness h , these inter-sensor temperature differences decrease, suggesting a more uniformly distributed thermal field over the contact length.

At higher cutting speeds and larger chip thicknesses, the recorded temperature signals exhibit increased scatter, transient fluctuations, and reduced signal stability. These effects limit the reliability of steady-state temperature evaluation under such conditions. Consequently, data points affected by signal instability were excluded from subsequent quantitative analysis to ensure consistency and robustness of the evaluated trends.

Steady-State Analysis in Rotary Orthogonal Cutting

The limited engagement time in linear orthogonal tests, ranging from 25 ms at $v_c = 120$ m/min to 100 ms at $v_c = 30$ m/min, restricts the assessment of steady-state conditions, particularly for thermal analyses. To overcome this limitation, rotary orthogonal cutting experiments were performed using the configuration described in Section 4.5.2, which enables prolonged tool–workpiece contact durations.

Figure 5.2 illustrates the time-resolved signals of cutting force (F_c), passive force (F_p), and temperature measurements acquired from the tool–chip interface (T_{tfs}), tool body (T_t), and workpiece sub-surface (T_w). The force signals exhibit a rapid rise followed by a plateau, indicating the establishment of mechanical steady-state conditions within the initial engagement phase. Conversely, the thermal response presents distinct dynamics. Both T_{tfs} and T_t stabilise after an initial transient, while T_w continues to rise throughout the cutting operation.

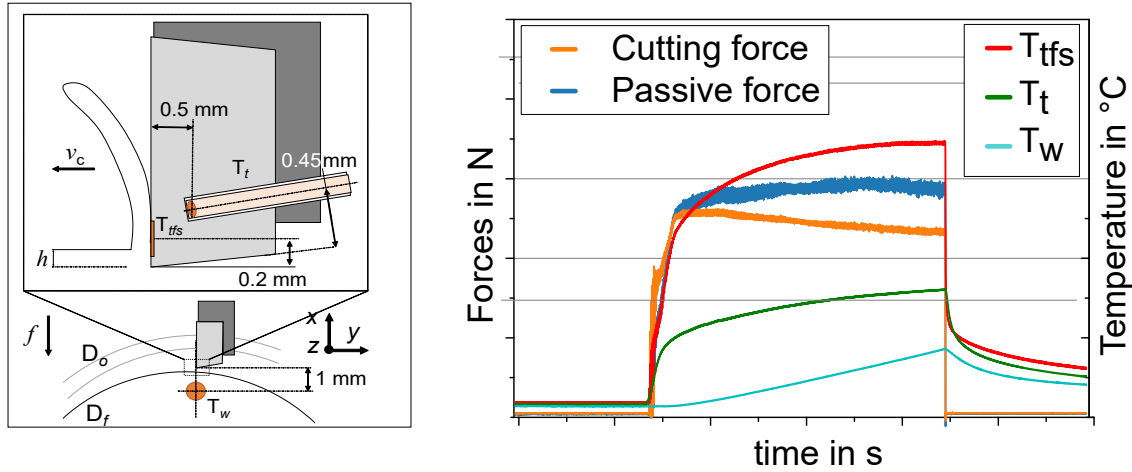


Figure 5.2: Time evolution of cutting force, passive force, and temperature signals during rotary orthogonal cutting. Thermal stabilisation occurs for T_{tfs} and T_t , while T_w exhibits continued rise due to cumulative heating.

The saturation of T_{tfs} and T_t indicates that thermal equilibrium is achieved locally at the tool level, thereby justifying the application of steady-state assumptions for subsequent thermal modelling. A quantitative convergence criterion was defined as a rate of change below 5% over a 50 ms time window. In contrast, the continuous increase of T_w is not indicative of thermal instability, but rather results from the geometric configuration of the rotary test. As material is progressively removed, the cutting zone approaches the fixed position of the thermocouple embedded in the workpiece, effectively reducing the distance to the heat source. Consequently, T_w rises steadily throughout the cut. For this reason, only the final temperature values recorded at the end of the test are considered representative of peak thermal exposure within the workpiece.

This spatially dependent behaviour highlights the importance of localised thermal measurements for accurately resolving transient and steady-state regimes in machining. Furthermore, the rapid stabilisation of mechanical signals relative to thermal ones confirms that thermomechanical equilibrium is reached on different timescales.

Figure 5.3 presents the evolution of cutting and passive forces as a function of uncut chip thickness for rotary orthogonal cutting trials at four cutting speeds. A pronounced increase in both force components is observed with rising h , reflecting the growing material engagement volume and consequent rise in shear load. This trend is most evident for F_c , which exhibits a steeper slope, particularly at lower cutting speeds, indicating its dominant role in governing energy dissipation through plastic deformation.

In the micro-scale cutting regime ($h \leq 50 \mu\text{m}$), the force behaviour departs from classical shearing models. Specifically, F_p approaches or even surpasses F_c , a signature of ploughing-

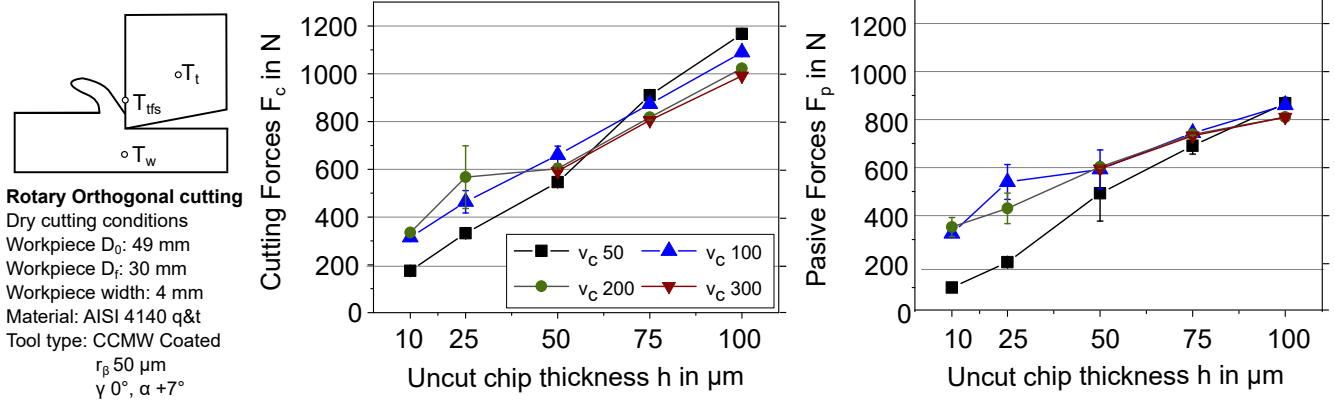


Figure 5.3: Cutting (F_c) and passive (F_p) forces as a function of uncut chip thickness h for various cutting speeds during rotary orthogonal cutting.

dominated contact mechanics, wherein the effective rake angle becomes negative due to the tool edge radius ($r_\beta = 50 \mu\text{m}$) being comparable to h . This effect amplifies compressive loading at the tool–workpiece interface, generating elevated normal stresses and contributing to the observed rise in F_p . Such conditions also promote material pile-up, adhesion, and edge rounding, leading to higher variability in the measured forces. Error bars are accordingly larger in this low- h regime, despite being averaged over three repetitions.

At higher uncut chip thicknesses ($h > 50 \mu\text{m}$), the deformation zone expands, and the forces increase more gradually. The curve's mild non-linearity suggests the influence of thermally activated mechanisms such as material softening and increased tool–chip sliding. A notable trend across all h values is the reduction in both F_c and F_p with increasing v_c . This behaviour is attributed to improved chip evacuation and localised thermal softening, which reduce the material's flow stress and facilitate deformation at higher cutting speeds.

Temperature Field and Peak Thermal Load Distribution

Figure 5.4 presents the spatial temperature distribution measured during rotary orthogonal cutting for two uncut chip thicknesses: $h = 50 \mu\text{m}$ and $h = 100 \mu\text{m}$. The profiles correspond to three distinct sensor signals: a thin-film sensor integrated into the tool rake face (T_{tfs}), an embedded thermocouple in the tool body (T_t), and another embedded thermocouple located within the workpiece (T_w). The temperature values plotted represent the maximum recorded by each sensor at the end of the cutting test, reflecting the quasi-steady thermal state achieved after prolonged tool–workpiece engagement.

Across all tests, the thin-film sensor (T_{tfs}) registers the highest temperatures, reaching values close to 650 °C at $h = 100 \mu\text{m}$. These peak temperatures indicate the dominant contribution of plastic deformation and intense friction at the tool–chip interface.

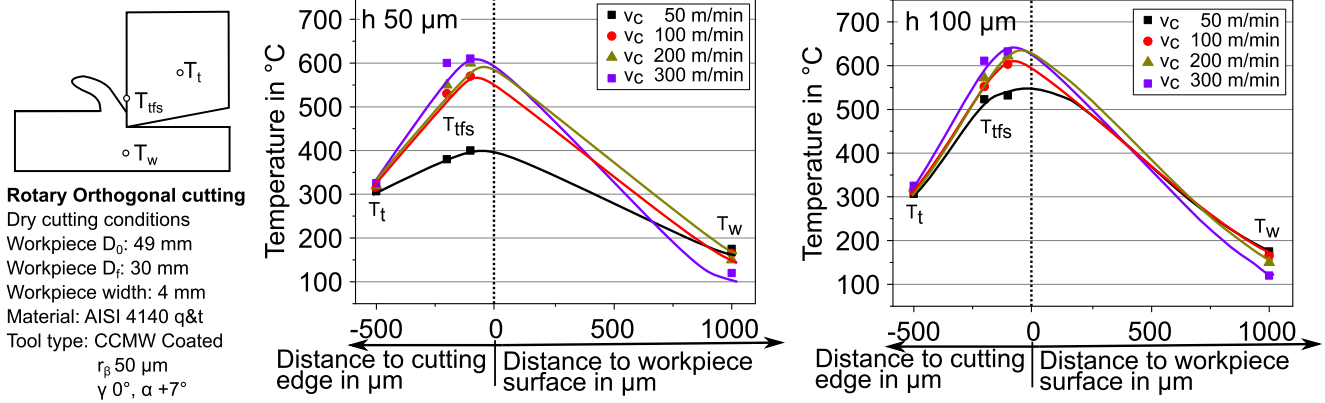


Figure 5.4: Maximum temperature distribution along the tool and workpiece surfaces.

In contrast, the tool- and workpiece-embedded thermocouples (T_t and T_w) report lower values due to their placement deeper within the thermal conduction path. This validates the effectiveness of the sensor placement in capturing localised thermal effects versus bulk heat transport. With increasing chip thickness, a significant rise in peak temperatures is observed for all sensors. This behaviour is attributed to the greater plastic work and frictional dissipation associated with higher material removal rates. Additionally, the steepening of thermal gradients at $h = 100 \mu$ m suggests increasingly localised heating with limited lateral heat conduction, confirming the reduced thermal diffusion length under high-load conditions.

A distinct thermal response is seen in the workpiece sensor (T_w), which does not exhibit saturation but instead shows a continuous increase in temperature along the cutting path. This cumulative heating behaviour is explained by the geometry of the rotary setup: as material is progressively removed, the workpiece diameter decreases, reducing the local cross-sectional area and, consequently, the material's thermal capacity and dissipation efficiency.

Another notable trend emerges when examining the influence of cutting speed. At higher speeds, the tool-related temperatures (T_{tfs} and T_t) increase significantly, whereas T_w exhibits only a moderate rise or even a tendency to plateau. This observation is consistent with prior findings in the literature (Childs & Maekawa et al. 2000) and is indicative of a shift in heat partitioning mechanisms at elevated cutting velocities. Specifically, the increased chip velocity enhances convective heat removal via the chip, thereby diverting a larger portion of the generated heat away from the workpiece and into the tool or surrounding air.

This partitioning favours elevated tool temperatures and aligns with the reduction in flow stress due to thermal softening at the interface, thereby lowering the cutting forces observed under such conditions.

5.1.2 Strain and Strain-Rate Tensors

Local strain and strain-rate fields were determined using high-speed digital image correlation (DIC) in the linear orthogonal cutting setup described in Section 4.5.1. Representative displacement fields, shown in Figure 5.5, reveal a sharply localised deformation band ahead of the tool edge, consistent with the primary shear zone of orthogonal cutting. The localisation of displacements marks the region of intense plastic shear, which is further analysed through the extracted strain and strain-rate tensors.

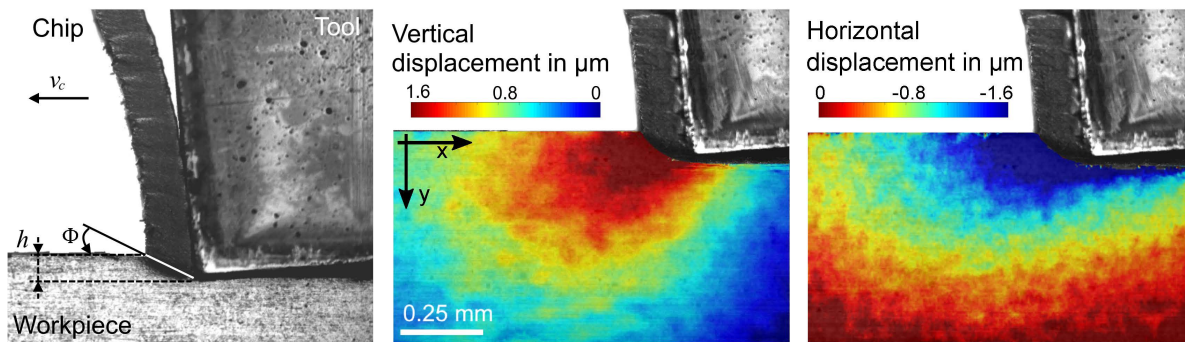


Figure 5.5: In-situ high-speed imaging and DIC post-processing: (a) raw high-speed image; (b) displacement fields in Y and X . Test conditions: $v_c = 120$ m/min, $h = 100$ μ m.

The DIC processing delivered full-field strain components ε_{xx} , ε_{yy} , and $2\varepsilon_{xy}$, together with the equivalent strain ε_{eq} , as summarised in Figure 5.6. Across all test conditions, deformation is dominated by shear: $2\varepsilon_{xy}$ is consistently the largest component, confirming that material flow is governed by concentrated shearing along an inclined primary shear band. The corresponding equivalent strains ($\varepsilon_{eq} \approx 2-4$) lie within the typical range reported for AISI 4140 under severe plastic deformation.

The strain and strain-rate fields extracted from DIC show a clear and consistent dependence on cutting speed and uncut chip thickness. Across all three values of h , the shear strain $2\varepsilon_{xy}$ is the dominant component, and its magnitude—together with the effective strain ε_{eq} —increases monotonically with cutting speed. This behaviour reflects the mechanics of the primary deformation zone (PDZ), where higher cutting speeds generate larger shear-strain rates and promote thermal softening, leading to a more localised shear band and consequently higher accumulated deformation. The corresponding strain-rate components exhibit the same trend: both $\dot{\varepsilon}_{eq}$ and, in particular, the shear-rate $2\dot{\varepsilon}_{xy}$ rise strongly with increasing v_c , consistent with the reduction of PDZ thickness and the intensification of plastic flow at high speed.

An increase in uncut chip thickness amplifies all strain and strain-rate measures. Larger h reduces the shear angle and increases the shear-plane length, which results in higher shear

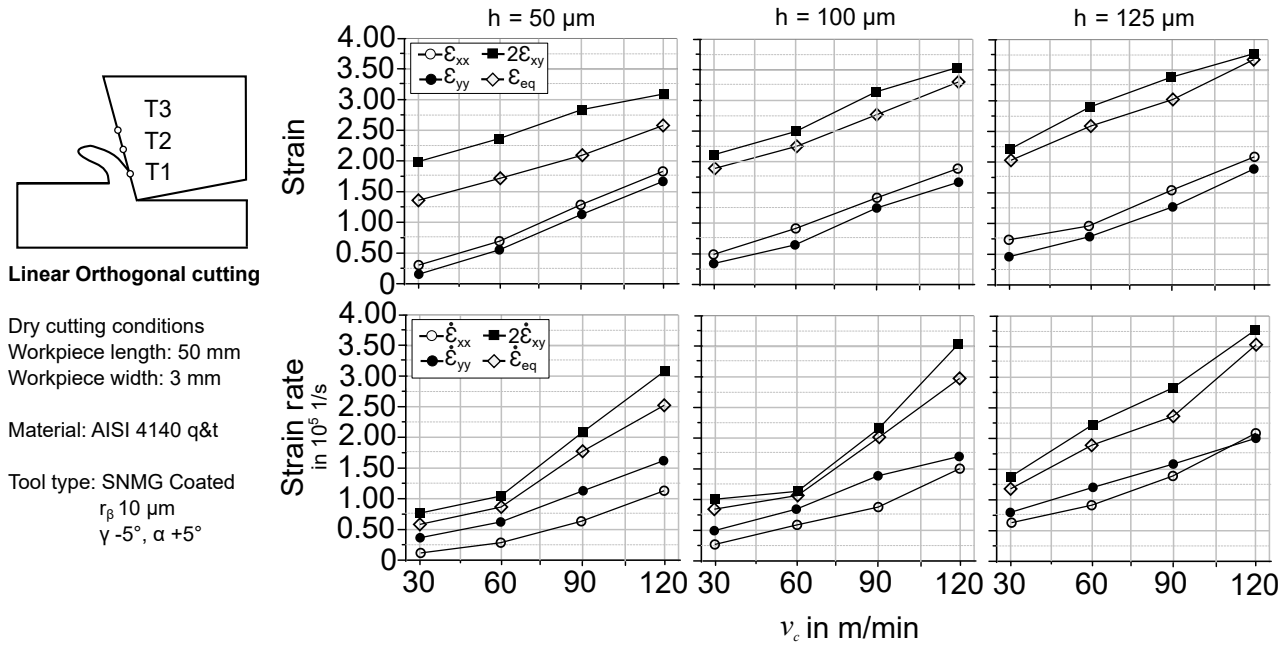


Figure 5.6: Measured in-plane strains (ε_{xx} , ε_{yy}), shear strain ($2\varepsilon_{xy}$), equivalent strain (ε_{eq}), and corresponding strain rates obtained from DIC.

strain and enhanced deformation-rate levels for otherwise identical cutting conditions. The combined effects of (i) speed-dependent shear localisation and (ii) the geometric influence of chip thickness produce the systematic and physically consistent trends observed in the figure. These experimentally derived strain and strain-rate fields therefore provide a robust deformation basis for calibrating the dislocation-density DRX model. The relative magnitudes of strain and strain-rate components show asymmetry. While ε_{xx} consistently exceeds ε_{yy} , the strain rate $\dot{\varepsilon}_{yy}$ occasionally surpasses $\dot{\varepsilon}_{xx}$. This can be attributed to transient compressive deformation beneath the chip–tool interface, where localised normal strains evolve on short time scales, producing elevated instantaneous strain rates despite moderate accumulated strain. The finite-difference time differentiation applied in DIC further amplifies such rapid temporal variations, especially in regions with steep gradients.

The spatial resolution of the DIC setup was approximately 2 μ m per pixel, while the temporal resolution of the high-speed camera was 10 μ s (100 kfps). The displacement uncertainty remained below 0.2 μ m across the field of view, corresponding to an average strain uncertainty of ± 8 –10% in regions of homogeneous deformation. Strain-rate values carry an additional uncertainty of approximately ± 15 % due to temporal discretisation and numerical differentiation. Although the extreme shear zone close to the chip–tool interface could not be fully resolved due to occlusion and motion blur, the measurable strain and strain-rate levels are consistent with published DIC studies and with the mechanistic understanding of chip formation in steels.

5.1.3 Tool–Chip Contact Length Evolution

The tool–chip contact length L_c is a key indicator of the load transfer and heat-flux concentration along the tool rake face during orthogonal cutting. It governs frictional energy input, chip sliding–sticking behaviour, and local surface integrity evolution. In this study, L_c was extracted directly from the high-speed imaging. The approach enables a quantitative, spatially resolved determination of the chip–tool interface length from the displacement field gradients and tracked chip flow kinematics under dry cutting conditions.

Figure 5.7a summarises the measured variation of L_c for different cutting speeds and chip loads, while Figure 5.7b shows example frames highlighting the chip–tool interface used to determine the contact length.

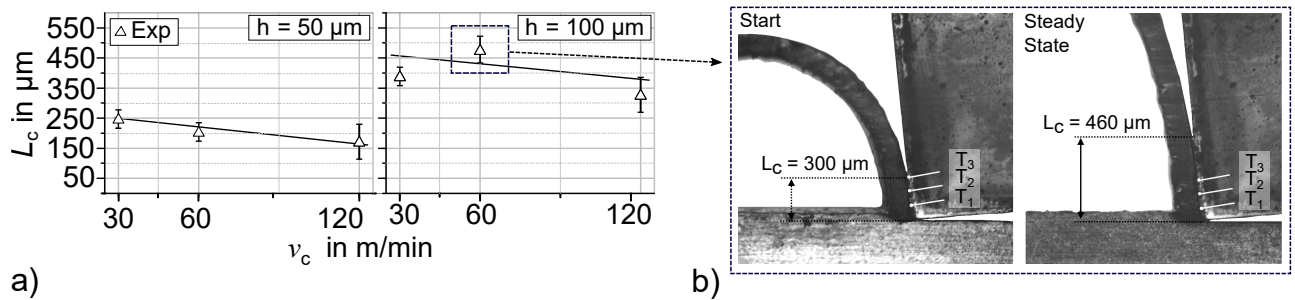


Figure 5.7: Tool–chip contact length L_c obtained from high-speed image analysis at different cutting speeds and uncut chip thicknesses: (a) quantitative evolution of L_c as a function of cutting speed; (b) representative measured contact region during chip formation (start and steady state).

A pronounced dependence of the tool–chip contact length L_c on uncut chip thickness was observed. At low chip load ($h = 50 \mu\text{m}$), the contact length was approximately $300 \mu\text{m}$, increasing to $\sim 460 \mu\text{m}$ for $h = 100 \mu\text{m}$. This increase can be attributed to the larger chip cross-section and the resulting geometric expansion of the tool–chip contact zone on the rake face at higher uncut chip thicknesses, rather than to a modification of the overall shear mechanism.

In contrast, increasing cutting speed at constant h led to a systematic decrease in L_c . For example, at $h = 100 \mu\text{m}$, increasing v_c from 50 to 120 m/min resulted in a reduction of approximately 10–15%. While this behaviour deviates from classical analytical models that predict a mild increase of contact length with cutting speed, it is consistent with experimental observations reported for dry cutting conditions. The decrease in L_c with increasing v_c is associated with changes in the thermomechanical state at the tool–chip interface, which promote shorter effective contact lengths without altering the overall shear geometry.

The measured contact-length trends reflect two distinct influences: increasing uncut chip thickness leads to a geometrically larger contact zone, whereas increasing cutting speed is associated with a reduction in the effective tool–chip interaction length. These observations provide an experimental basis for the contact conditions considered in the subsequent analysis.

5.1.4 Hardness

Subsurface hardness is a key indicator of machining-induced surface integrity, reflecting the combined influence of strain hardening and thermal softening. Depth-resolved hardness profiles were obtained by microindentation following linear orthogonal cutting, using the same cutting conditions analysed for strain and contact-length evaluation. Figure 5.8 presents the evolution of subsurface hardness as a function of uncut chip thickness and cutting speed. The profiles reveal distinct regimes of material response, reflecting the competition between plastic deformation-induced hardening and temperature-driven softening.

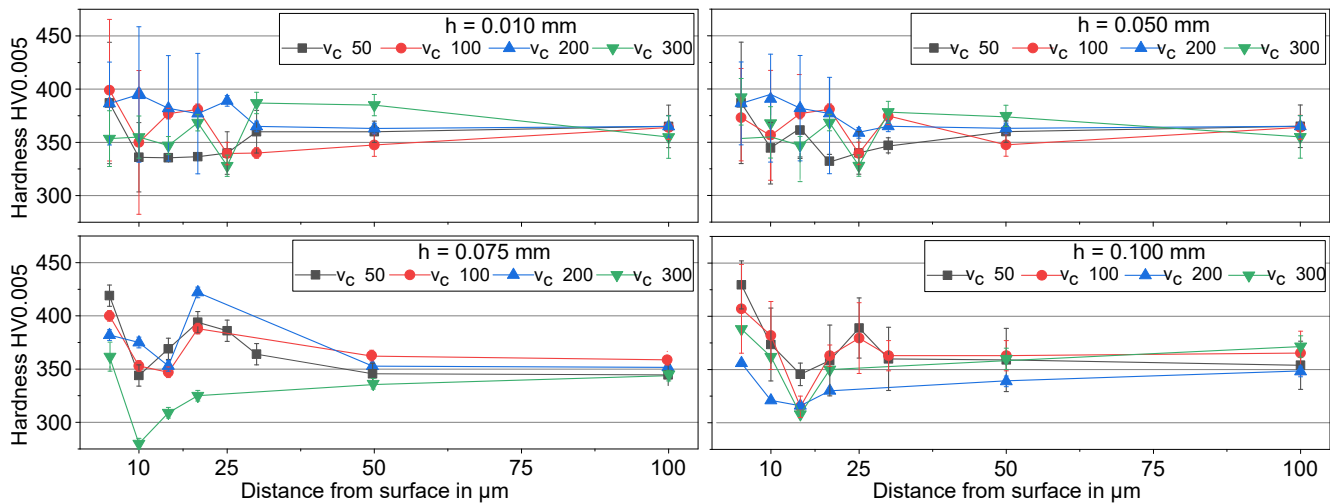


Figure 5.8: Depth-dependent hardness for varying uncut chip thicknesses ($h = 10$ – 100 μm) and cutting speeds ($v_c = 50$ – 300 m/min) in rotary orthogonal cutting.

At the lowest chip load ($h = 10$ μm), a pronounced subsurface hardening peak of approximately 430 HV_{0.005} is observed at a depth of 15–25 μm. This hardening is characteristic of ploughing-dominated cutting, where the uncut chip thickness approaches the tool edge radius and induces severe subsurface deformation beneath the tool.

Increasing the uncut chip thickness to $h = 50$ – 75 μm results in a dual-layer hardness response. A hardened near-surface zone is retained, while a local softening region develops at depths of approximately 30–50 μm. This subsurface softening coincides with regions exposed to elevated temperatures during cutting and is attributed to thermally activated

recovery processes, leading to a partial reduction in dislocation density below the hardened layer.

At the highest chip load ($h = 100 \mu\text{m}$), the hardness gradient becomes less pronounced and the peak hardness values decrease. Under these conditions, the combined influence of high cutting speed ($v_c \geq 200 \text{ m/min}$) and prolonged thermal exposure promotes thermal softening effects that counteract strain hardening, resulting in a more uniform subsurface hardness distribution.

Scatter in the indentation data reflects both intrinsic heterogeneity within the plastically affected zone and the measurement sensitivity associated with small indentation depths. Variability is most pronounced in the ploughing regime (low h), where material flow and surface roughness are highly non-uniform. Maximal hardening occurs when intense plastic strain is not fully counteracted by thermal recovery, whereas higher chip loads and cutting speeds lead to a mixed response governed by concurrent strain accumulation and temperature rise.

5.1.5 Dislocation Density from X-ray Line-Profile Analysis

Cutting-induced lattice distortion was quantified by X-ray diffraction (XRD) line-profile analysis on AISI 4140 specimens prepared under four reference conditions: (i) a quenched-and-tempered baseline, (ii) an induction-hardened state, (iii) a shot-peened surface provided by IAM-KIT, and (iv) dry machining under rotary orthogonal cutting at $v_c = 200 \text{ m/min}$ and $h = 100 \mu\text{m}$ using three nominally identical coated cemented-carbide inserts.

Figure 5.9(a) shows the instrument-corrected full width at half maximum (FWHM, β) of selected Bragg peaks as a function of the scattering vector $s = 2 \sin \theta / \lambda$. The quenched-and-tempered baseline exhibits the narrowest diffraction peaks, with representative FWHM values of approximately $5 \times 10^{-3} \text{ \AA}^{-1}$, corresponding to a dislocation density in the range of $(0.8\text{--}1.2) \times 10^{15} \text{ m}^{-2}$.

Induction hardening results in a marked increase in peak broadening, with FWHM values approximately 40% higher than the baseline. Shot peening produces the largest peak broadening among all reference conditions, providing an upper bound for mechanically induced lattice distortion.

Dry machining leads to intermediate peak broadening, with $\beta \approx 1.3 \times 10^{-2} \text{ \AA}^{-1}$, corresponding to dislocation densities in the range of $(3.8\text{--}4.5) \times 10^{15} \text{ m}^{-2}$. The results obtained from the three cutting inserts are closely clustered, indicating good reproducibility of the machining-induced microstructural state.

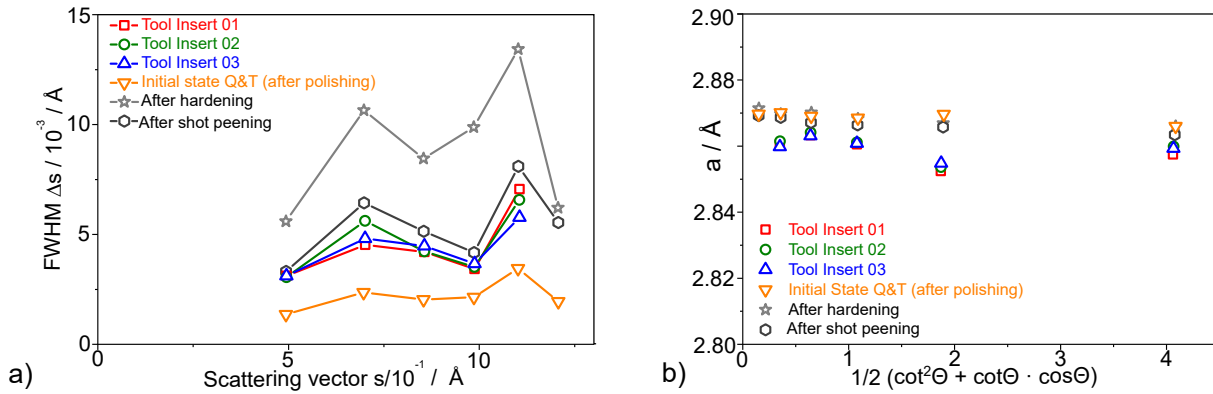


Figure 5.9: Williamson–Hall evaluation of AISI 4140 for different material and processing conditions: (a) instrument-corrected FWHM broadening β as a function of scattering vector s ; (b) corresponding modified Williamson–Hall representations. Results for the quenched-and-tempered state, induction-hardened condition, and shot-peened surface are shown for reference. Machining results correspond to rotary orthogonal cutting using three nominally identical tool inserts.

The dislocation densities measured after dry machining lie between those of the induction-hardened and shot-peened reference conditions, indicating substantial but non-saturating lattice distortion in the near-surface region. These experimentally derived values are used as quantitative calibration targets for the physically based constitutive models employed in the subsequent simulation studies. Residual stress effects were not considered; only line-broadening contributions associated with lattice distortion were evaluated.

5.1.6 Microstructure: Grain Size

Machining imposes concurrent thermal and mechanical loads that drive dynamic recrystallisation (DRX) and, consequently, alter surface integrity. Grain refinement was therefore quantified on cross-sections prepared by focused ion-beam (FIB) milling, while complementary nano-indentation and XRD data were used to correlate hardness and dislocation density with the observed microstructure. The FIB images were segmented differentiating an ultrafine-grained layer (Section I, $d < 0.1 \mu\text{m}$) from an underlying grain-refined layer (Section II, $d < 1 \mu\text{m}$).

Figure 5.10 shows that DRX depth is non-monotonic. A maximum total thickness of $\sim 3.8 \mu\text{m}$ occurs at the intermediate setting $v_c = 200 \text{ m/min}$, $h = 50 \mu\text{m}$. Neither the highest speed nor the largest chip load produced the deepest refined layer, underscoring the need for a balanced thermomechanical regime.

At moderate conditions, plastic work and heat generation are sufficient, and exposure times long enough, to activate grain-boundary migration. Increasing the speed to 300 m/min raises

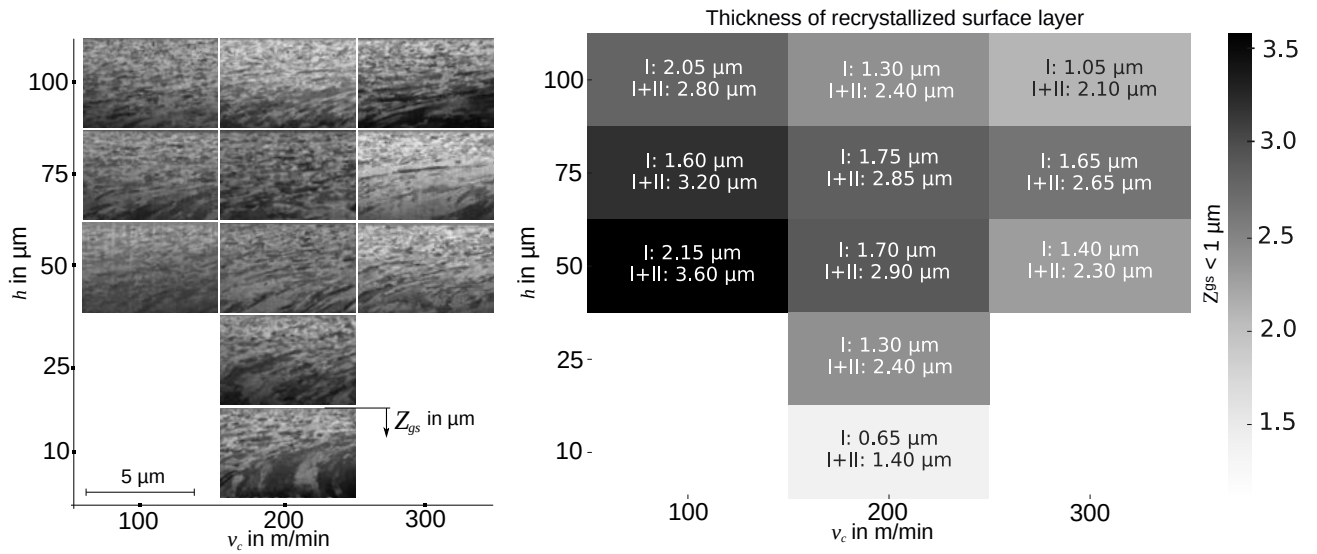


Figure 5.10: Thickness of dynamically recrystallised layers obtained by FIB for varying cutting speeds v_c and uncut chip thicknesses h . Section I: $d < 0.1 \mu\text{m}$; Section I+II: $d < 1 \mu\text{m}$. Rotary orthogonal cutting, dry, AISI 4140, insert CCMW 1204xx.

interface temperature but simultaneously shortens contact time and enhances chip-borne heat removal, limiting subsurface heat accumulation and suppressing DRX depth. Force data (Fig. 5.3) corroborate this: a thermal-softening-induced drop in cutting force at high v_c indicates lower mechanical work per unit volume and reduced driving pressure for recrystallisation.

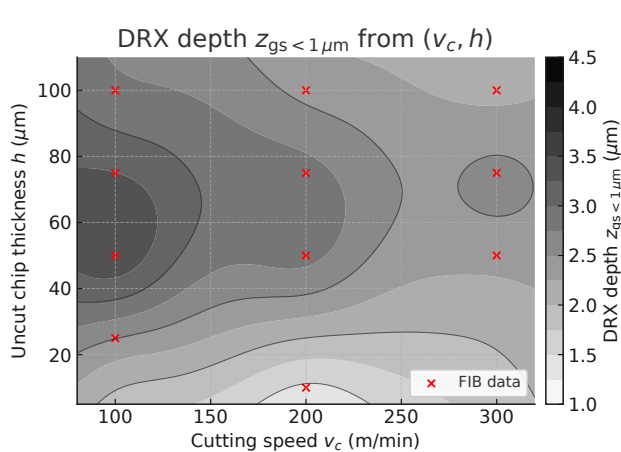
The smallest chip load ($h = 10 \mu\text{m}$) shows negligible refinement at all speeds. Here, ploughing dominates because the tool-edge radius approaches the chip thickness, producing high compressive stress but insufficient shear strain to trigger DRX. Peak grain refinement is achieved not under maximum heat or maximum strain alone, but where strain rate, temperature, and contact duration act synergistically. This interpretation provides a direct microstructural link between the hardness evolution and the dislocation-density trends observed in the preceding sections.

5.1.7 Regression-Supported Microstructure Interpretation

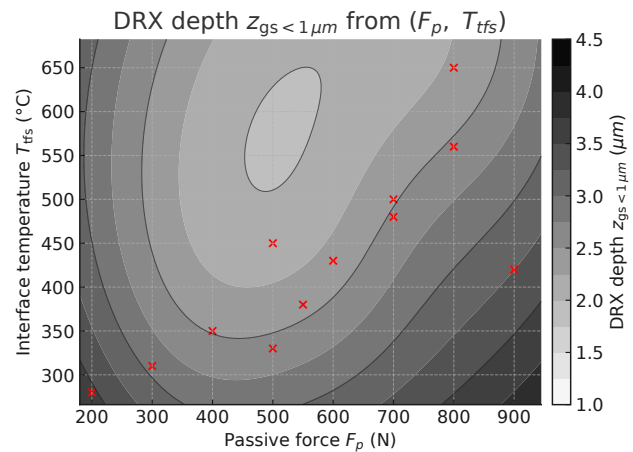
Using a radial basis function (RBF) interpolation, two surrogate models were constructed to examine whether empirical response surfaces can capture the experimentally observed evolution of the dynamically recrystallised layer. Two predictor sets were evaluated: nominal process parameters (v_c, h) and in-process quantities (F_p, T_{tfs}). The resulting response surfaces are shown in Figure 5.11, where subfigures (a) and (b) correspond to (v_c, h) and (F_p, T_{tfs}), respectively. Red crosses indicate the experimental FIB measurements used as interpolation anchors.

Figure 5.11(a) captures the experimentally observed behaviour with a distinct maximum DRX depth of approximately $3.5\text{--}4.0\ \mu\text{m}$ located around $v_c = 150\text{--}200\ \text{m/min}$ and $h = 50\ \mu\text{m}$. This reflects the interplay between plastic strain accumulation, heat generation, and contact duration. At intermediate cutting speeds, both mechanical work and thermally activated processes contribute to grain-boundary migration, while the dwell time of the tool–workpiece interface remains long enough for heat to diffuse into the subsurface. At higher speeds, increased chip evacuation and reduced interaction time suppress subsurface heat accumulation despite elevated surface temperatures, leading to lower DRX depths. Conversely, very small uncut chip thicknesses ($h \leq 25\ \mu\text{m}$) result in ploughing-dominated deformation with insufficient shear strain to trigger DRX, yielding minimal refinement. Taken together, the surface reflects the expected coupling between strain rate, temperature, and exposure time governing subsurface microstructural evolution in dry orthogonal cutting.

Figure 5.11(b) employs in-process signals, passive force F_p and interface temperature T_{tfs} , as predictors. These quantities are directly measurable during machining and therefore attractive candidates for soft-sensor development. The interpolated surface displays broad plateaux and localised maxima centred around $F_p \approx 500\text{--}600\ \text{N}$ and $T_{\text{tfs}} \approx 600\ ^\circ\text{C}$, consistent with the optimum region identified in panel (a). This regime corresponds to the conditions under which both energetic deformation (via strain energy) and thermal activation coexist, enabling grain boundary migration and DRX. At lower force/temperature combinations, the energy input is insufficient for grain refinement, while excessively high temperatures tend to reduce DRX depth, likely due to dynamic recovery effects coupled with shorter contact durations that limit sustained dislocation accumulation.



(a) Interpolation using process parameters



(b) Interpolation using forces and temperatures

Figure 5.11: Interpolated maps of the dynamically recrystallised layer thickness $z_{\text{gs} < 1\ \mu\text{m}}$. Red crosses indicate the locations of experimental FIB/SEM measurements used as anchor points for the interpolation.

However, fine details in Figure 5.11(b) must be interpreted cautiously. Strong correlation between F_p and T_{tfs} , combined with sparse sampling in the high-load region, introduces uncertainty in the RBF interpolation. The apparent “double-peak” feature does not necessarily indicate two distinct physical regimes; rather, it reflects artefacts caused by variable collinearity and limited experimental data density. These limitations underscore the challenge of relying solely on empirical regressors to describe microstructural evolution in a strongly coupled thermomechanical process.

Small datasets, even when interpolated with smooth RBF kernels, are insufficient to ensure robust predictive behaviour across changes in tool geometry, material state, or process stability. The (F_p, T_{tfs}) -based interpolation remains valuable for qualitative assessment and for developing sensor-based monitoring strategies but requires augmentation by physics-based constraints or hybrid modelling to achieve predictive reliability. Consequently, the next Section (Section 5.2) presents the results of the two-dimensional finite-element simulations, which implement constitutive behaviour and microstructure-evolution laws.

This physics-based modelling framework enables controlled extrapolation beyond the experimentally accessible parameter space while maintaining mechanistic fidelity. The FEM results therefore provide a more robust foundation for predicting DRX depth and machining-induced surface integrity than purely empirical regression alone.

5.2 2D Finite Element Simulation Results

This section presents the outcomes of the two-dimensional finite element simulations conducted to investigate the thermomechanical response of orthogonal cutting under dry conditions. The simulations were designed to capture the effect of machining parameters on key surface integrity indicators such as stress, temperature, strain, and strain rate, while abstracting the turning process to a simplified 2D orthogonal cutting configuration under plane strain. The modelling approach, detailed previously in Section 4.6, neglects tool wear and focuses on the steady-state regime to isolate the intrinsic material response. The simulation setup, boundary conditions, and constitutive models were selected to replicate the dry orthogonal experiments and enable quantitative comparison.

The results presented herein provide insight into subsurface gradients, chip formation dynamics, and the spatial evolution of physical fields, which form the basis for subsequent microstructure modelling and regression-based surrogate development. Particular emphasis is placed on understanding how uncut chip thickness and cutting speed modulate thermomechanical loads at the tool–workpiece interface and drive microstructural transformations in the near-surface region.

5.2.1 Results of Force-Based Johnson–Cook Calibration

This section presents the outcome of the Johnson–Cook (JC) material model calibration described in Section 4.6.5. The model was parametrised using force measurements obtained from rotary orthogonal cutting tests (Fig. 5.3) and a multistep quasi-stationary FEM strategy. Four cutting conditions were selected as calibration points, and the JC parameters were iteratively adjusted to minimise the root-mean-square deviation between simulated and measured cutting (F_c) and passive forces (F_p). Figure 5.12 compares simulated and experimental forces for all tested machining conditions. Calibration points are explicitly indicated, while all other cases serve as independent validation of the model.

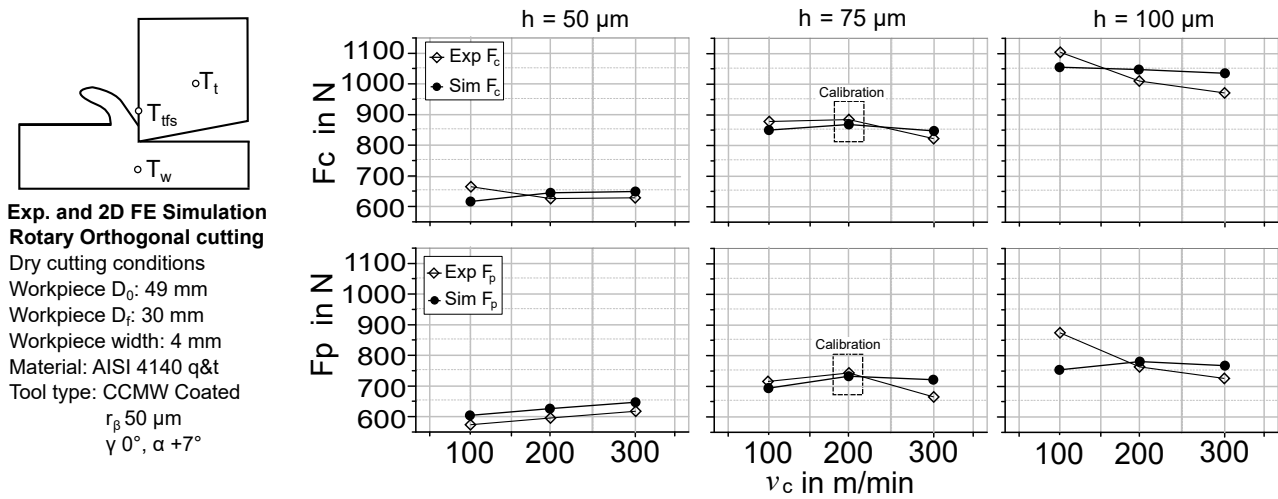


Figure 5.12: Comparison of simulated and experimental cutting (F_c) and passive (F_p) forces over the investigated machining conditions.

The JC model accurately reproduces the principal force trends across the test matrix. In particular, the nonlinear increase of both F_c and F_p with uncut chip thickness h is well captured, reflecting the enlarged deformation volume and associated rise in shear-plane load. The experimentally observed decrease in force with increasing cutting speed v_c is also reproduced, although the simulated reduction is slightly less pronounced. This minor deviation may stem from the simplified strain-rate sensitivity and thermal softening formulation intrinsic to the classical Johnson–Cook model.

No calibration or validation tests were conducted at uncut chip thicknesses smaller than the cutting-edge radius (i.e., $h < 10 \mu\text{m}$). Such conditions are dominated by ploughing, size effects, and potential build-up edge formation, which are challenging to capture within a conventional 2D Lagrangian FEM framework.

5.2.2 Thermal Model Calibration Using Tool Temperature Gradients

Following the force-based calibration of the JC material model, the thermal boundary conditions of the 2D FEM model were adjusted using temperature measurements obtained from orthogonal cutting experiments. Thermal calibration was performed within the quasi-steady multistep simulation strategy described in Section 4.6.1, focusing on validating the mechanical response under the modified tool geometry and subsequently tuning heat-transfer parameters to match the measured temperature gradients. Prior to thermal fitting, simulated forces were compared with experiments to ensure the JC model remained valid under the linear orthogonal configuration.

Figure 5.13 compares the calibrated FEM temperatures and forces against experiments for uncut chip thicknesses of $h = 50 \mu\text{m}$ and $h = 100 \mu\text{m}$. The calibrated thermal parameters are: Effective heat-transfer coefficient: $h_{\text{sink}} \approx 6200 \text{ W m}^{-2} \text{ K}^{-1}$, and Heat-sink thermal conductivity: $k_{\text{sink}} \approx 85 \text{ W m}^{-1} \text{ K}^{-1}$. These values fall within typical ranges reported for metallic tool–holder assemblies and represent effective parameters that include contact resistances, coating effects, and system-scale conduction paths.

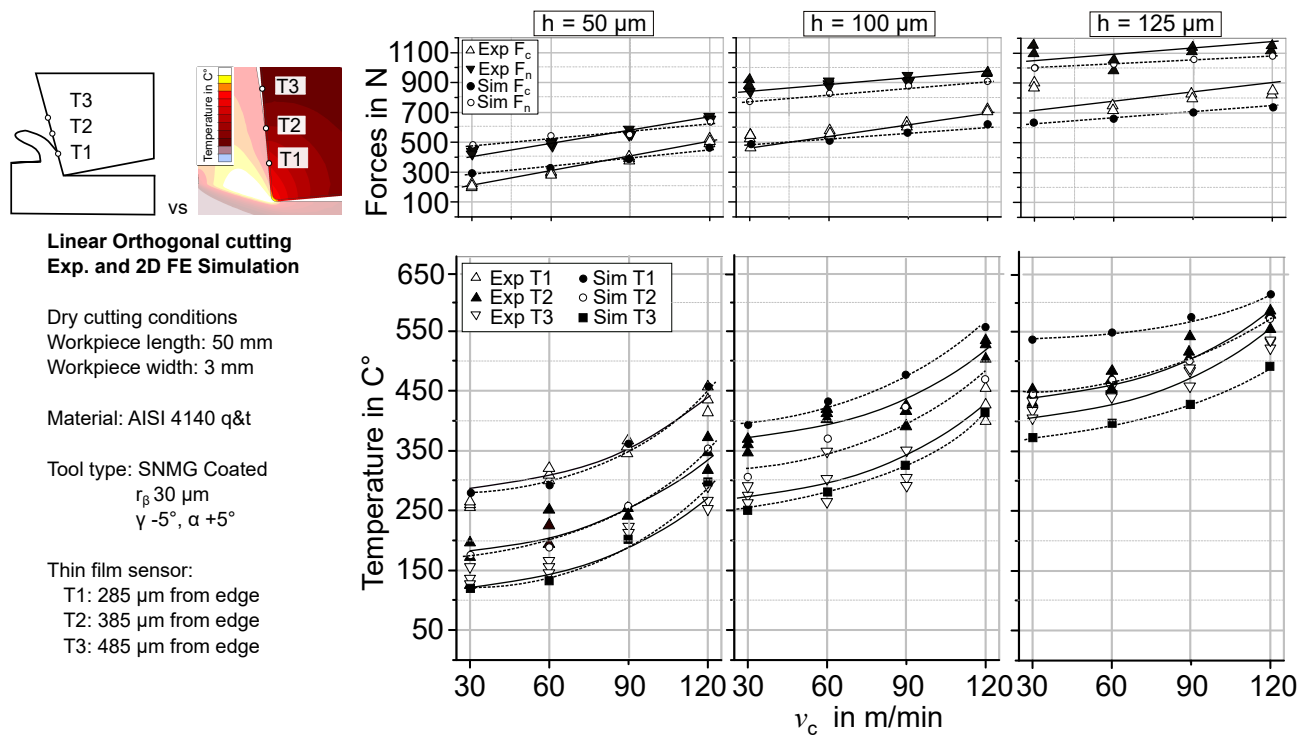


Figure 5.13: Comparison of experimental and simulated cutting forces and rake-face temperatures during linear orthogonal cutting.

Deviations in F_c and F_p remained below 5 %, confirming consistency between the rotary and linear setups. The thermal model was then calibrated by adjusting two effective parameters: (i) the heat-transfer coefficient at the tool–heat sink interface h_{sink} , and (ii) the thermal conductivity

of the heat sink body k_{sink} . These parameters were iteratively tuned to minimise the root-mean-square deviation between measured and simulated temperatures at the three sensor locations. In the FEM model, sensor positions were mirrored using Lagrangian tracers embedded at identical distances from the cutting edge. Unlike studies that impose fixed heat-partitioning ratios, this work derives heat flow directly from FEM-resolved heat fluxes at the chip, tool, and workpiece boundaries. For the calibrated conditions, the partitioning of total generated heat has been summarised in Table 5.1, together with other values from benchmark literature, confirming the physical consistency of the calibrated thermal model.

Table 5.1: Heat-partitioning ratios during dry orthogonal cutting of steel.

Source	Chip (%)	Tool (%)	Workpiece (%)
Komanduri & Hou (2001)	60–75	10–20	10–20
Childs et al. (2000)	60–70	15–25	10–15
Arrazola et al. (2013)	65	20	15
Ozel et al. (2006)	66	22	12
This study	64	21	15

5.2.3 DRX Model Calibration and Selection

The calibrated thermomechanical fields obtained from the 2D FEM framework were used to evaluate the three decoupled dynamic recrystallisation formulations introduced in Section 4.6.4: (i) a Zener–Hollomon (ZH) type model, (ii) a Helmholtz free-energy based model, and (iii) a dislocation-density (DD) based model. All models were applied during the final refinement stage of the quasi-steady orthogonal cutting simulation, in which the element size in the primary shear zone was reduced to $0.5 \mu\text{m}$ to resolve the steep gradients of strain, strain rate and temperature that drive DRX. The resulting qualitative grain-refinement fields are shown in Figure 5.14. Regions coloured blue correspond to fully recrystallised material with $d < 1 \mu\text{m}$, whereas red regions represent material that retains its initial microstructure.

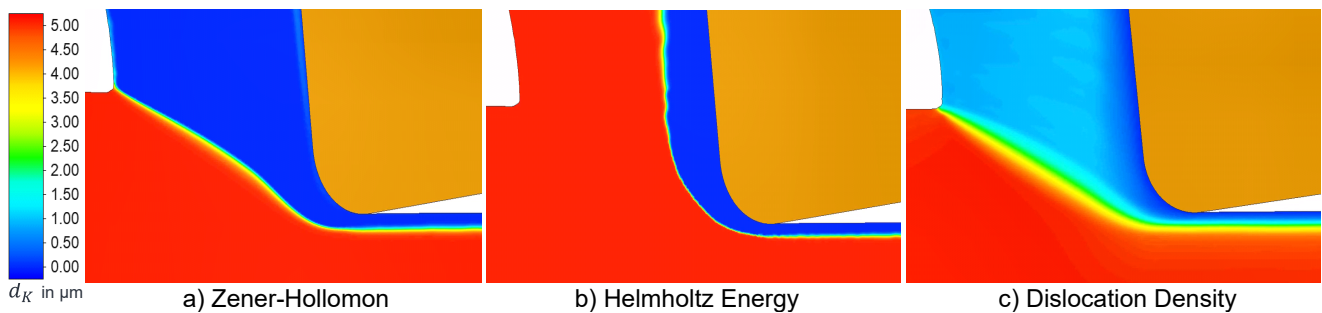


Figure 5.14: Qualitative chip-region grain refinement predicted by the three DRX models for dry orthogonal cutting ($v_c = 100 \text{ m/min}$, $r_\beta = 110 \mu\text{m}$, $h = 30 \mu\text{m}$).

The Zener–Hollomon model produces a comparatively sharp transition between recrystallised and non-recrystallised regions, reflecting its threshold-type activation with strong dependence on the Z -parameter. The Helmholtz free-energy model yields a more diffuse DRX front and generally overestimates the recrystallised area due to its sensitivity to mechanical energy dissipation. In contrast, the dislocation-density model predicts smooth spatial gradients and a gradual transition from fully to partially recrystallised material, consistent with the coupled evolution of dislocation storage, dynamic recovery and DRX nucleation. This behaviour aligns more closely with the experimentally observed microstructural transitions in the chip and subsurface regions. To quantify model performance, the recrystallised depth $Z_{d=1\mu\text{m}}$ was evaluated for a wide range of tool form factors $\kappa = r_\beta/h$. The results are shown in Figure 5.15, together with experimental measurements from the rotary orthogonal cutting tests.

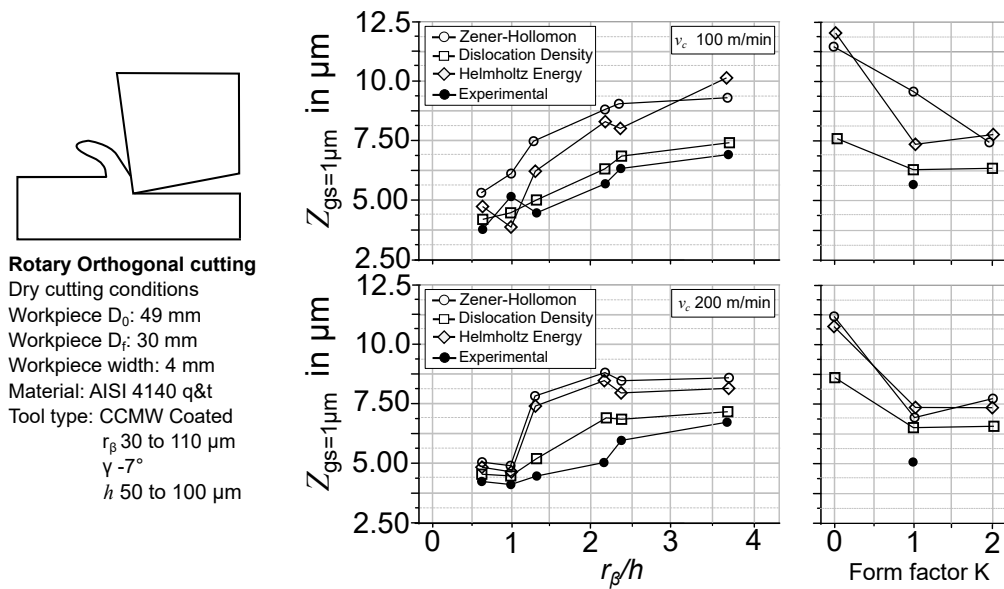


Figure 5.15: Variation of recrystallised layer depth $Z_{d=1\mu\text{m}}$ with form factor $\kappa = r_\beta/h$. Comparison of experimental measurements with predictions from the Zener–Hollomon, Helmholtz free-energy and dislocation-density DRX models.

For both cutting speeds, the recrystallised depth exhibits a minimum at intermediate form factors $\kappa \approx 1$, where the edge radius and uncut chip thickness are of comparable magnitude and subsurface deformation beneath the edge is most intense. At small values of κ , corresponding to sharp tools, DRX depth decreases because shear is concentrated in a relatively thin primary zone with limited subsurface penetration. At large κ , the process becomes increasingly ploughing-dominated; although local strains remain high, the effective shear strain in the near-surface layer decreases and dynamic recovery is enhanced, leading again to reduced recrystallised depth. Across all cutting conditions, the dislocation-density model provides the closest agreement with the experimental data, typically within 25%. The Zener–Hollomon model consistently underpredicts the DRX depth due to its strong Z -dependence and lack of

recovery mechanisms, whereas the Helmholtz free-energy formulation tends to overestimate DRX, particularly at higher κ . Based on these observations, the dislocation-density model was selected for subsequent use in the 3D FEM simulations and in the soft-sensor framework described in Section 4.8.

Validation Against In-situ High-Speed DIC Measurements

The FEM deformation fields were first validated using high-speed DIC measurements obtained in the accessible region of the primary deformation zone (Section 4.2.2). Because optical access is limited to the near-surface and the zone immediately ahead of the shear band, FEM–DIC comparison was performed along Lagrangian material paths that coincide with the experimentally observable region.

Table 5.2 summarises the comparison for four cutting speeds. For all investigated conditions, the FEM-predicted strain and strain-rate magnitudes lie within the DIC uncertainty bounds ($\pm 10\%$ for strain and $\pm 15\%$ for strain rate). In particular, the dominant shear component $2\varepsilon_{xy}$ is accurately reproduced, confirming that the FEM correctly captures the kinematics of the primary shear zone. This agreement provides confidence that the subsurface deformation fields predicted by the FEM, unobservable by DIC, are sufficiently accurate for subsequent DRX modelling.

Table 5.2: Comparison of FEM and DIC strain magnitudes for $h = 50 \mu\text{m}$ across four cutting speeds.

v_c (m/min)	Component	DIC	FEM	Deviation (%)	Note
30	ε_{xx}	0.30	0.28	6.7	within tolerance
	ε_{yy}	0.20	0.19	5.0	within tolerance
	$2\varepsilon_{xy}$	2.00	1.85	7.5	shear-dominated
	ε_{eq}	1.45	1.38	4.8	—
60	ε_{xx}	0.75	0.70	6.7	—
	ε_{yy}	0.50	0.46	8.0	—
	$2\varepsilon_{xy}$	2.30	2.15	6.5	—
	ε_{eq}	1.80	1.72	4.4	—
90	ε_{xx}	1.25	1.18	5.6	—
	ε_{yy}	1.15	1.09	5.2	—
	$2\varepsilon_{xy}$	2.75	2.60	5.5	—
	ε_{eq}	2.50	2.38	4.8	—
120	ε_{xx}	1.80	1.70	5.6	—
	ε_{yy}	1.60	1.52	5.0	—
	$2\varepsilon_{xy}$	3.10	2.90	6.5	—
	ε_{eq}	3.35	3.20	4.5	—

FEM–Experiment Validation of DRX Depth

Figure 5.16 compares the refined grain layer depth $Z_{d<1\mu\text{m}}$ predicted by the calibrated dislocation-density DRX model with corresponding FIB/SEM measurements across the investigated (v_c, h) process window. The right-hand panel shows the FEM-based interpolated contour map, with simulated values indicated by open circles and experimental FIB/SEM measurements marked by red triangles.

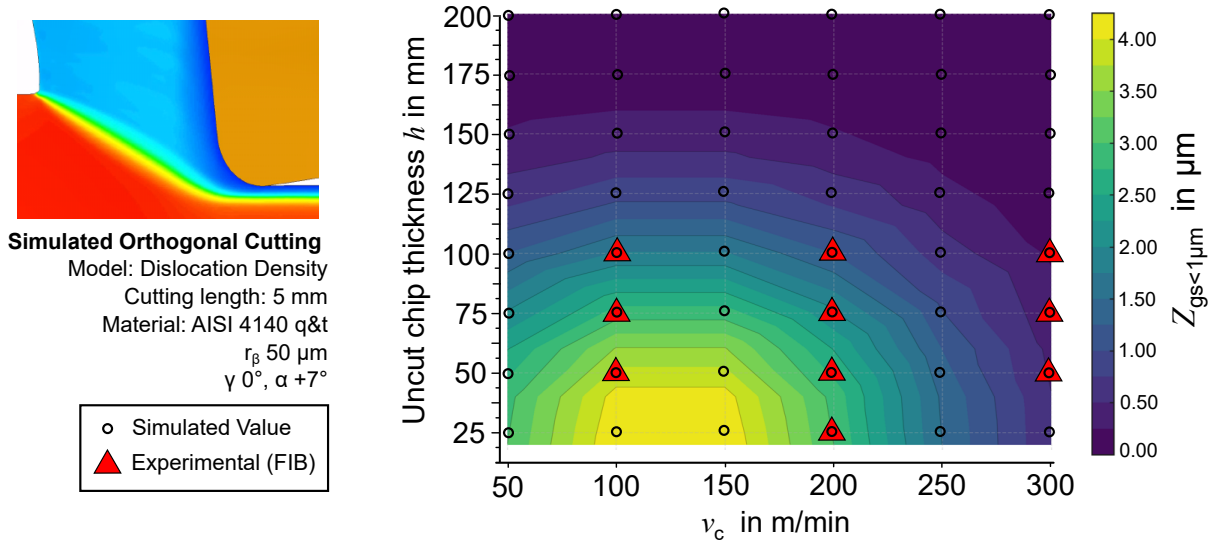


Figure 5.16: Refined grain layer depth $Z_{d<1\mu\text{m}}$ predicted by the dislocation-density DRX model as a function of cutting speed v_c and uncut chip thickness h for dry orthogonal cutting of AISI 4140. The contour map represents interpolated FEM predictions; open circles indicate simulated values and red triangles denote experimental FIB/SEM measurement locations.

The model reproduces the experimentally observed dependence of DRX depth on process parameters. The interpolated DRX depth exhibits a local maximum at intermediate chip thicknesses ($h \approx 50\text{--}75\ \mu\text{m}$), while reduced DRX depths are observed at both small and large chip thicknesses. With increasing cutting speed, the DRX depth increases up to approximately $v_c \approx 150\ \text{m/min}$, beyond which no further increase is observed within the investigated range.

Quantitatively, the deviation between simulated and experimental DRX depths remains below 30% across the full parameter space. Larger deviations occur primarily for very shallow DRX layers, where the experimental depth resolution of FIB/SEM becomes limited, and at high cutting speeds where the predicted DRX response is sensitive to strain-rate-dependent thermal softening. Despite these local deviations, the simulations reproduce the correct order of magnitude and scaling of DRX depth with respect to cutting speed and uncut chip thickness.

5.3 Discussion

The results presented in this chapter demonstrate that two-dimensional finite element modelling, when consistently calibrated against cutting forces, temperatures, and DIC-derived deformation fields, can reproduce the dominant mechanical and thermomechanical mechanisms governing chip formation and near-surface microstructural evolution in AISI 4140 under dry orthogonal cutting. The combined use of thin-film temperature sensing, high-speed DIC, and a quasi-steady FEM framework enables a physically consistent reconstruction of the local deformation and thermal fields within the primary and secondary deformation zones.

A key outcome of this work is the quantitative reconciliation of experimentally measured surface strain fields with subsurface FEM strain predictions. By mapping numerical strain histories at subsurface locations corresponding to optically accessible regions in the experiments, direct comparison with DIC data becomes possible despite the inherent limitations of optical access in the shear zone. The observed agreement confirms the physical consistency of the calibrated FEM fields and provides a reliable basis for microstructure-resolved post-processing.

Using these validated thermomechanical histories, three decoupled dynamic recrystallisation formulations were evaluated. The comparison revealed substantial differences in predicted grain refinement, underlining the necessity of physically grounded DRX models for machining applications. Among the investigated approaches, the dislocation-density-based formulation showed the highest predictive capability, accurately reproducing both the magnitude and the parametric dependence of experimentally measured DRX depths on cutting speed and uncut chip thickness.

The limitations inherent to two-dimensional orthogonal cutting simulations must nevertheless be acknowledged. Effects associated with out-of-plane deformation, chip curl, successive tool engagements, and cumulative thermal loading cannot be captured within a 2D framework and may lead to an underestimation of recovery processes at larger depths of cut or during multi-pass machining. In addition, strong gradients in the vicinity of the rounded cutting edge remain sensitive to numerical interpolation despite careful mesh refinement.

Within these constraints, the presented framework establishes a robust and physically consistent basis for microstructure-informed machining analysis. The integration of experimentally validated thermomechanical fields with mechanistic DRX modelling enables quantitative surface integrity prediction and provides a direct transition toward the three-dimensional simulations addressed in the following chapter, where realistic tool trajectories, chip flow geometries, and fully three-dimensional thermal fields relevant to industrial machining are considered.

6 Results of Longitudinal Turning Processes

6.1 Experimental Results

The following sections present the experimental observations obtained from the longitudinal turning tests. The objective is to quantify how feed, depth of cut, and cutting speed influence force generation, thermal loading at the tool–chip interface, wear progression, and the resulting surface integrity. All tests were performed under dry conditions using CCMT-120408 inserts as introduced in section 4.5.3. The results form the basis for validating the thermo-mechanical fields predicted by the 3D simulations discussed in the subsequent chapter.

6.1.1 Cutting Forces

The cutting, feed, and passive force components exhibit clear and systematic dependencies on feed rate, depth of cut, and cutting speed. Higher feed levels and larger engagement areas increase the material removal load and lead to correspondingly higher force magnitudes, whereas the sensitivity to cutting speed remains comparatively small. These relationships are quantified in Fig. 6.1, which compiles the measured forces across all tested parameter combinations. Each row represents one feed level ($f = 0.1, 0.2$, and 0.3 mm/rev), while the three columns show the individual force components. For each feed, the three depths of cut ($a_p = 0.3, 0.6, 1.2$ mm) appear distinctly separated in all panels, demonstrating consistent scaling behaviour. The error bars indicate the standard deviation across repeated measurements and confirm high experimental repeatability. Increasing the feed from 0.1 to 0.3 mm/rev produces a substantial increase in F_c and F_f , reflecting the larger chip cross-section and enlarged shear plane. The near-proportional scaling is characteristic of stable chip formation and aligns with classical orthogonal cutting mechanics. The depth of cut further amplifies all force components, particularly F_c , and the approximately linear rise in force magnitude with a_p confirms the absence of chatter or intermittent chip formation. A slight reduction in F_c and F_f with increasing cutting speed is observed for all parameter sets. This effect is most noticeable at higher feed and depth-of-cut levels, where thermal softening in the primary shear zone becomes more relevant. The magnitude of this reduction remains moderate, which is consistent with the strong heat conduction into the carbide tool. The passive force F_p shows a distinct behaviour. While F_p increases with feed and depth of cut, it remains largely unaffected by cutting speed. This indicates that passive loading is dominated by normal stresses on the flank face rather than by shear-zone mechanics. Only minor reductions at higher cutting speeds appear in selected cases. At the most aggressive settings ($f = 0.3$ mm/rev, $a_p = 1.2$ mm), F_p exceeds 200 N, underlining the importance of flank–workpiece contact in determining tool load.

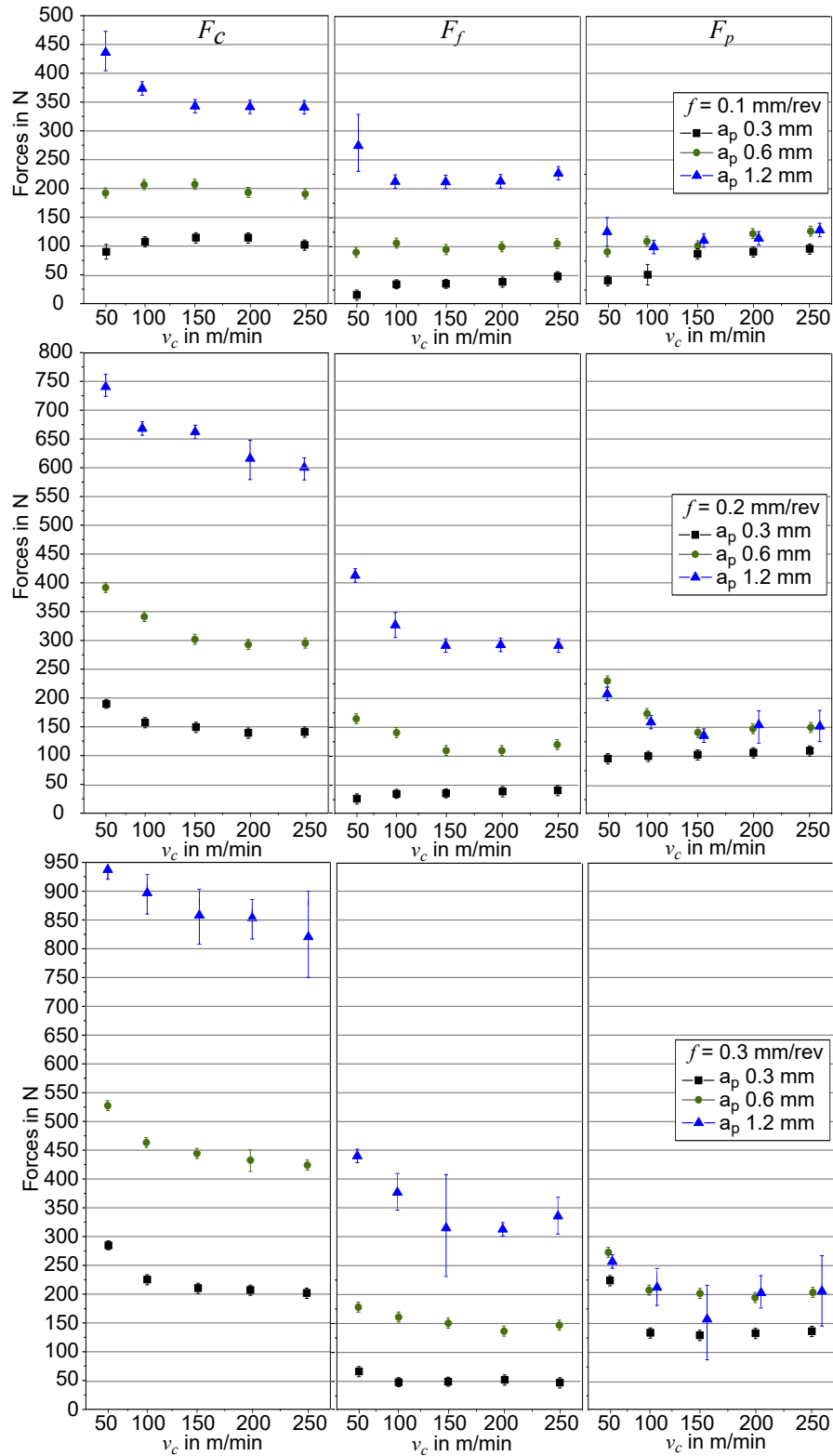


Figure 6.1: Measured cutting (F_c), feed (F_f), and passive (F_p) forces as a function of cutting speed v_c for different feed rates and depths of cut using CCMT-120408-FK6 inserts.

6.1.2 Cutting Temperatures

The thermal response at the rake face reflects the combined mechanical and frictional processes governing chip formation. The thin-film sensors embedded in the insert, as introduced in Fig. 4.21, enable local monitoring of the tool-internal temperature field and provide insight into the influence of cutting speed and feed on heat flow into the carbide body.

The temperature–time curves in Fig. 6.2 exhibit an initial rapid temperature increase followed by a quasi-steady regime, defined here as the time interval in which the rate of temperature increase becomes small compared to the initial heating transient. For the cutting speeds investigated in Fig. 6.2a, this quasi-steady behaviour is observed for TM1 approximately between $t \approx 4$ –8 s, while TM2 reaches a comparable regime at lower absolute temperature levels due to its larger distance from the cutting edge.

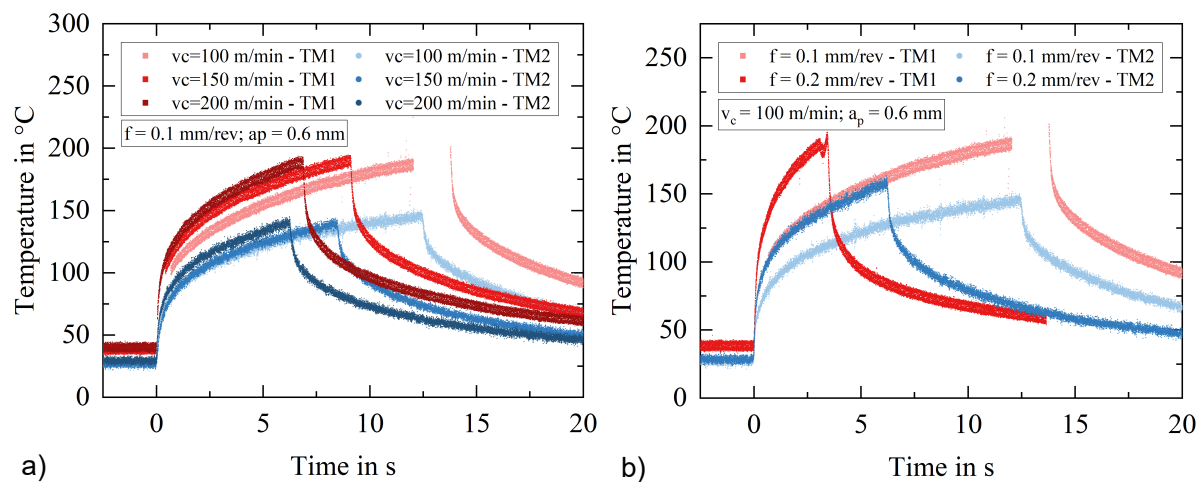


Figure 6.2: Temperatures measured with thin-film sensors during turning tests. (a) Effect of cutting speed at constant feed. (b) Effect of feed rate (Plogmeyer & González et al. 2024).

During the quasi-steady regime, a balance is established between the heat conducted into the carbide insert and the heat removed by the chip and the workpiece, resulting in a slowly varying tool-internal temperature despite continued heat generation at the tool–chip interface. The temperature measured at the sensor location therefore stabilises in a practical sense, even though the true interface temperature is expected to exhibit significantly higher values and short-wavelength fluctuations that are strongly attenuated within the tool.

The effect of cutting speed is illustrated in Fig. 6.2a. Although increasing cutting speed raises the rate of heat generation at the interface, the tool-internal temperature field changes only moderately because the thermal gradient inside the insert remains largely unchanged. TM1, located closer to the cutting edge, responds more rapidly and reaches a higher quasi-

steady temperature level, while TM2 remains largely insensitive to short-wavelength thermal fluctuations originating at the interface.

At higher feed rates, the TM1 signal collapses before a quasi-steady regime is reached. This behaviour indicates mechanical overloading of the thin-film sensor stack caused by increased cutting and passive forces (cf. Fig. 6.1). Likely failure mechanisms include local delamination of the insulating layer, cracking of the substrate beneath the sensor, or rupture of the metallic thermoresistive track due to bending or compressive stresses. This signal collapse highlights the strong coupling between thermal and mechanical loading in the near-edge region and delineates the operational limits of sensor survivability under aggressive cutting conditions.

Both thin-film sensors are positioned well beneath the tool–chip interface. At this distance, the measured temperatures represent a strongly attenuated form of the interfacial thermal field. The high thermal conductivity of cemented carbide, combined with the short characteristic time for heat diffusion within the insert, leads to a steep temperature gradient near the cutting edge. Consequently, the sensor outputs primarily reflect the bulk heat flow into the tool rather than the flash temperatures and rapid thermal fluctuations present in the primary shear zone.

Because surface integrity is governed by the local thermomechanical conditions within a few micrometres of the workpiece surface, tool-internal temperature measurements cannot be used to infer microstructural modification directly. However, they provide an essential constraint for numerical modelling. The measured quasi-steady temperature levels, the heating transients, and the time required to reach this regime impose stringent boundary conditions on the heat partition between chip, tool, and workpiece in the FEM simulations.

6.1.3 Tool Wear

The progression of flank wear (VB) governs both the mechanical load acting on the tool and the stability of the cutting process. Differences in insert geometry and chip–tool interaction lead to distinct wear evolution patterns, which ultimately control the onset of accelerated abrasion and tool failure. Figure 6.3 shows the temporal development of VB for the MP6 and RK6 geometries at $f = 0.20$ mm/rev and $a_p = 1.2$ mm. The corresponding tool geometries are shown in Fig. 4.20.

Across all tests, wear progressed predominantly as uniform abrasive flank wear, with no measurable crater wear or edge chipping. This behaviour is typical for hardened AISI 4140, where abrasion dominates over brittle fracture mechanisms. As the wear land increased, the enlarged flank–workpiece contact zone amplified the ploughing component of the cutting process, which is reflected in the experimentally observed increase of the passive force

F_p (Section 6.1.1). This establishes a direct link between wear progression and increasing normal stresses in the tertiary deformation zone.

For the MP6 geometry, flank wear exhibited a strong dependence on cutting speed. At $v_c = 150$ m/min, VB increased steadily and approached approximately 150 μm after 50 minutes of cutting time, after which the growth rate began to flatten. At $v_c = 200$ m/min, wear continued to increase throughout the test and reached roughly 200 μm . At higher cutting speeds ($v_c = 250$ – 300 m/min), wear progression became distinctly non-linear, with a pronounced acceleration during the later stages of cutting, ultimately leading to premature tool failure before the target cutting time was reached. This accelerated wear is attributed to elevated local stresses and thermal loading induced by the chip-breaker geometry, which promotes chip segmentation and increases normal contact pressures near the cutting edge.

For the RK6 geometry, tests were restricted to $v_c = 250$ and 300 m/min due to unstable chip evacuation at lower cutting speeds caused by the absence of a chip breaker. In contrast to MP6, the plain rake face of RK6 promotes continuous chip flow and a more distributed chip–tool contact. Under otherwise identical cutting conditions, the RK6 insert exhibits a slower progression of flank wear compared to MP6, with lower VB values over the entire cutting time.

The reduced wear rate of RK6 is attributed to the absence of chip-breaker–induced stress concentration on the rake face. The smoother chip flow leads to a more uniform distribution of contact stresses and mitigates localised thermal and mechanical loading at the cutting edge. Consequently, although chip control is less effective for RK6, the flank wear progression remains more gradual than for the MP6 geometry.

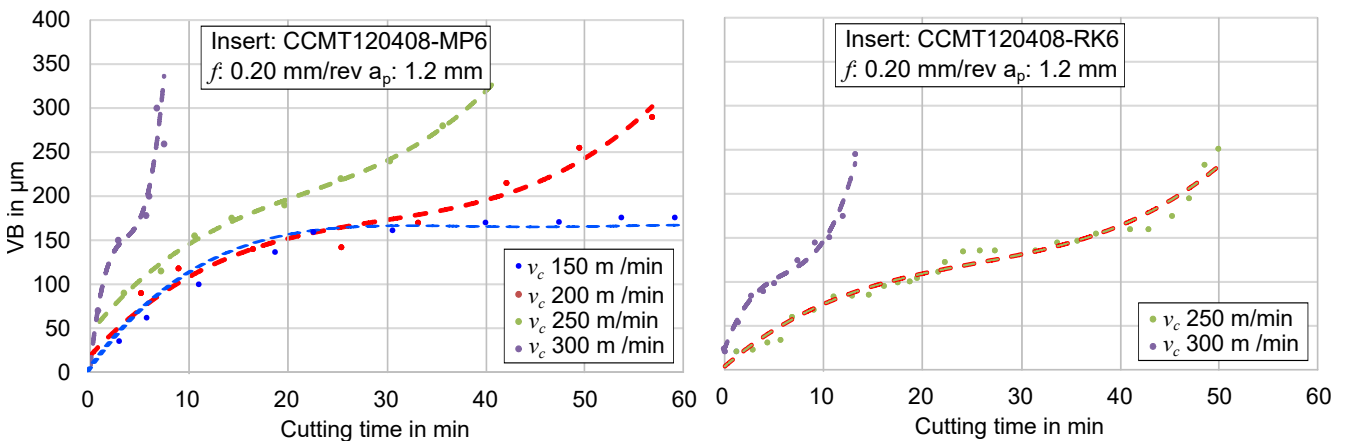


Figure 6.3: Tool wear progression during longitudinal turning for MP6 and RK6 insert geometries at $f = 0.20$ mm/rev, $a_p = 1.2$ mm and different v_c .

6.1.4 Surface Integrity

The evolution of surface integrity is governed by the combined mechanical and thermal loading transmitted through the flank face. As abrasive wear widens the wear land, the conditions in the tertiary deformation zone change fundamentally: the local normal stresses increase, contact length grows, and frictional dissipation becomes more significant. These mechanisms collectively intensify the severe plastic deformation (SPD) and dynamic recrystallisation (DRX) processes responsible for forming the ultrafine-grained (UFG) surface layer. The coupled evolution of flank wear (VB), passive force (F_p), and UFG layer thickness (z_{gs}) is summarised in Fig. 6.4.

At the beginning of tool life ($VB \approx 0$), the flank–workpiece contact is minimal, and the passive force remains comparatively low. Under these conditions, the surface layer experiences deformation primarily from the primary and secondary shear zones, resulting in a UFG layer of approximately $1.2 \mu\text{m}$. This refined layer reflects strain localisation at high strain rates, where DRX is activated but confined to a shallow region near the surface.

As flank wear progresses, the widening wear land substantially modifies the local stress and temperature fields. Figure 6.4 shows that once VB exceeds roughly $150 \mu\text{m}$, the passive force begins to rise non-linearly. This increase is a direct consequence of enhanced ploughing and longer real contact length along the flank face. The intensified mechanical loading acts directly on the material in the tertiary deformation zone, where the surface is repeatedly compressed under high hydrostatic stress and elevated frictional heating. These conditions are ideal for promoting DRX.

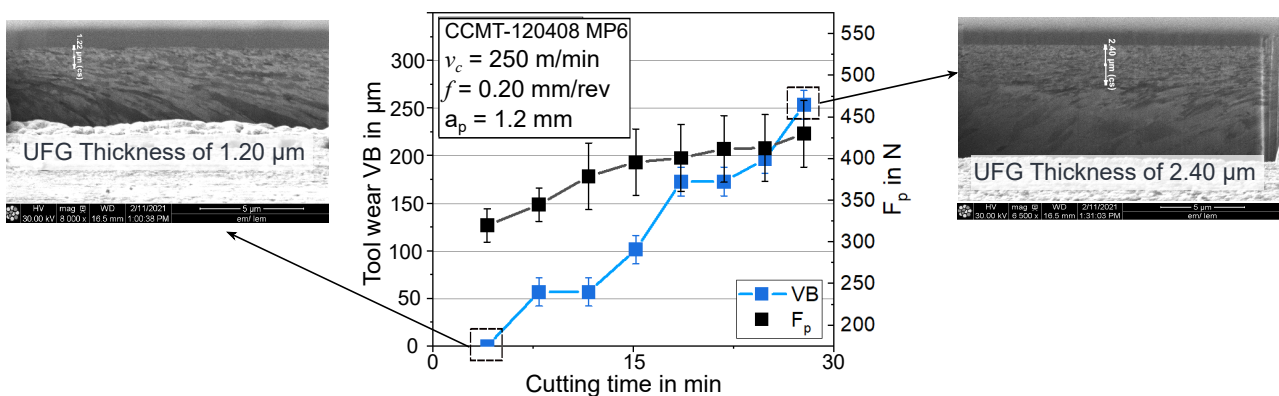


Figure 6.4: Relationship between flank wear (VB), passive force (F_p), and UFG surface layer thickness during longitudinal turning.

When VB reaches approximately $250 \mu\text{m}$, F_p increases to nearly 500 N . At this stage, the combined effect of mechanical indentation and thermally assisted DRX results in a UFG layer

thickness of around $2.4\ \mu\text{m}$, approximately double that observed for the unworn tool. This reflects a deeper penetration of the DRX-active zone, driven by sustained high plastic strains and increased thermal softening near the surface. These results establish a clear mechanistic pathway linking abrasive flank wear to surface integrity modification. The passive force acts as the critical intermediary variable, capturing the severity of flank-face loading and correlating directly with the depth and intensity of the resulting UFG layer. The observed microstructural evolution is therefore best interpreted as a wear-driven, mechanically dominated process, modulated by thermally assisted DRX at elevated cutting speeds.

6.2 3D Finite Element Simulation Results

The 3D FEM simulations presented in this chapter build upon the modelling framework established in the 2D plane-strain configuration. In Section 4.6.4, the Johnson–Cook constitutive law and the dislocation-density-based DRX model were calibrated against orthogonal cutting experiments, providing a robust description of flow stress, thermal softening, and microstructural refinement.

While the 2D simulations captured the principal thermo-mechanical behaviour and reproduced force levels, temperatures, and DRX kinetics with good accuracy, their geometric simplifications, absence of tool nose radius, zero out-of-plane heat flow, and idealised flank contact limit their predictive capability for longitudinal turning. In particular, plane-strain formulations constrain the stress state to two dimensions and neglect lateral material flow around the tool nose, which leads to an underestimation of normal contact stresses on the flank face.

The absence of three-dimensional heat conduction further suppresses localised flash temperatures generated by frictional sliding and plastic dissipation at the tool–workpiece interface. As a consequence, the thermal and mechanical loading acting on the near-surface material is underestimated, and the simulated recrystallised layer remains too shallow and laterally uniform. These limitations prevent 2D models from reproducing the experimentally observed depth variation and curvature of the ultrafine-grained (UFG) surface layer in longitudinal turning.

The transition to the fully three-dimensional framework (Section 4.6.6) addresses these limitations. The 3D model incorporates (i) the true tool geometry including nose radius, chip-breaker features, and edge rounding; (ii) spatial heat conduction into the tool and workpiece, enabling lateral heat spreading and thermal shielding effects; (iii) out-of-plane chip flow and the resulting variation of contact pressure along the cutting edge; and (iv) the geometric influence of flank wear (VB) on ploughing load, normal contact stresses, and surface flash temperature. These aspects are essential for accurately predicting surface integrity and the strong wear sensitivity documented in Chapter 6, and cannot be represented in a 2D formulation. A further

advantage of the 3D approach is the multi-pass strategy (Section 4.6.6), which enables cumulative thermo-mechanical history effects to be represented. Temperature fields, plastic strain histories, stress components, and DD-predicted grain sizes are transferred between passes, allowing the tool to interact with material that has already been mechanically and microstructurally modified. This cumulative-history capability constitutes a central methodological contribution of this thesis and is crucial for modelling surface integrity under realistic production conditions.

These improvements come at a high computational cost. The 3D turning model consists of several million degrees of freedom, employs adaptive meshing to resolve steep gradients near the tool–chip interface, and requires long cutting lengths to reach quasi-steady chip formation. Depending on wear level and mesh density, individual simulations require tens to hundreds of CPU hours. For this reason, the simulations were conducted using a structured design of experiments covering representative cutting conditions.

Simulations were performed at $f = 0.20$ mm/rev, depths of cut $a_p = 0.3$ – 1.2 mm, and cutting speeds $v_c = 50$ – 300 m/min for three flank wear states $VB = 0, 150, \text{ and } 300$ μm . The resulting thermo-mechanical fields, temperatures, cutting forces, and microstructural predictions are compared directly to the experimental results presented in Section 6 and serve as the high-fidelity database underpinning the process maps and Bayesian wear-inference framework introduced in the subsequent chapter.

6.2.1 Thermal Fields

The predicted temperature distributions reveal strong localisation of heat at the rake face and within the primary shear zone. Peak temperatures in excess of 800°C are reached even at moderate cutting speeds, and steep thermal gradients form towards the workpiece bulk and the interior of the tool. These gradients arise from high local heat generation combined with efficient conduction into the tool and workpiece.

Figure 6.5 shows the thermal field for $v_c = 150$ m/min. The global view (Fig. 6.5a) illustrates the general heat accumulation near the rake and flank faces, while the magnified view (Fig. 6.5b) highlights the narrow primary shear zone where peak temperatures occur. These high-temperature regions form the thermal drivers for dynamic recrystallisation and surface grain refinement. Compared to the 2D model, the 3D simulations predict notably higher surface flash temperatures due to the incorporation of flank contact and realistic heat spreading into the chip-breaker region.

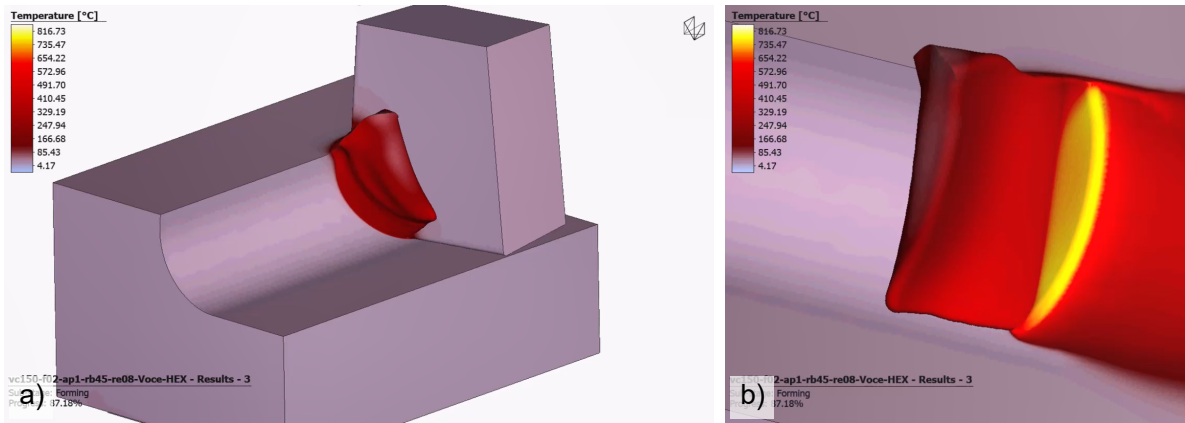


Figure 6.5: Temperature distribution in the workpiece and chip during 3D FEM cutting simulations at $v_c = 150$ m/min, $f = 0.20$ mm/rev, $a_p = 0.6$ mm. (a) Global temperature field highlighting heat localisation at the tool–chip interface. (b) Enlarged view of the primary shear zone showing peak temperatures exceeding 800°C .

6.2.2 Microstructural Predictions

The dislocation-density-based DRX model, applied in post-processing, provides detailed insight into the formation of the ultrafine-grained layer. Regions where $X_{\text{DRX}} \approx 1$ correspond to full dynamic recrystallisation and coincide spatially with grain sizes below 100 nm. These predictions reflect the combined influence of severe plastic deformation, high strain rates, and temperature. Because post-DRX grain growth is not modelled, the predicted grain sizes constitute lower-bound estimates of refinement. Figure 6.6 presents the DRX fraction and grain size distribution for $v_c = 150$ m/min.

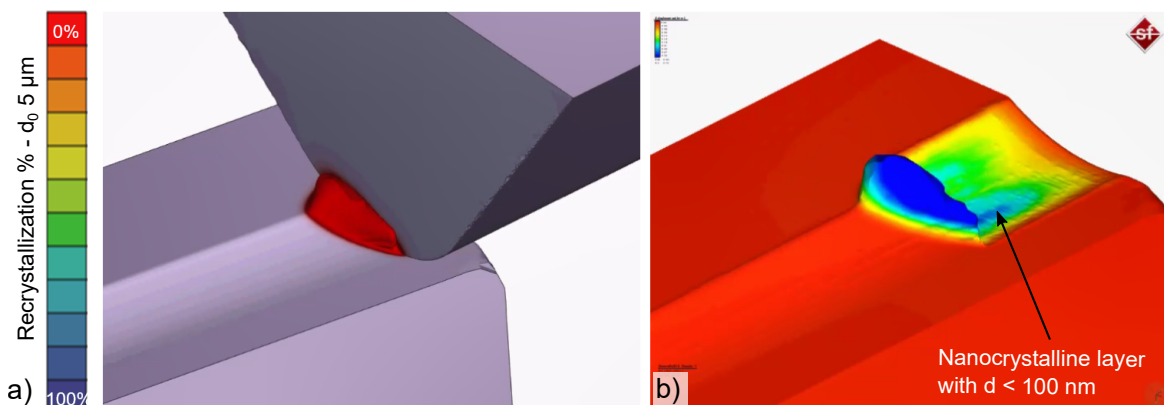


Figure 6.6: Microstructural predictions from the post-processed dislocation-density-based DRX model for $v_c = 150$ m/min. (a) Fraction of dynamically recrystallised grains X_{DRX} , where 100% indicates full recrystallisation in regions of extreme strain and temperature. (b) Corresponding grain size distribution showing the ultrafine-grained (nanocrystalline) layer where $d_f < 100$ nm. The UFG region is spatially coincident with $X_{\text{DRX}} \approx 1$.

The thickness and curvature of the recrystallised layer agree closely with the SEM cross-sections obtained experimentally. Compared to the 2D model, the 3D framework predicts a deeper and more strongly curved UFG layer, reflecting the influence of flank contact and the three-dimensional strain field on DRX activation.

6.2.3 Validation Against Experiments

The predictive capability of the 3D FEM model was assessed by comparing the simulated cutting forces, tool-side temperatures (T_{TF1}), and UFG layer thickness against the experimental dataset. Validation results for the unworn tool ($VB = 0 \mu\text{m}$) are summarised in Table 6.1, with corresponding results for $VB = 150$ and $300 \mu\text{m}$ provided in Tables 6.2 and 6.3. Errors remain below 7% for all quantities.

Three robust validation trends are observed:

- **Cutting forces:** Tangential (F_c) and passive (F_p) forces are reproduced within 2–7% across all speeds and wear states. The strong rise of F_p with flank wear is captured accurately.
- **Tool-side temperature:** T_{TF1} is predicted within 4–7% error, and its increase with v_c and VB matches the experimental response.
- **Microstructure:** UFG layer thickness $z_{gs < 1 \mu\text{m}}$ is predicted with errors typically below 6%, and the trend of increasing refinement with cutting speed and wear closely follows the SEM observations.

The FEM systematically overpredicts F_c by 1–3% and underpredicts F_p by 2–6%, suggesting a modest underestimation of normal stress on the flank. However, these discrepancies are small and do not affect the overall predictive trends.

Table 6.1: Validation for $VB = 0$: predicted vs. measured cutting forces, TF1 temperature, and UFG layer thickness at different speeds v_c . Relative error = $|Sim - Exp|/Exp \times 100\%$. T_{max} is simulation-only.

v_c (m/min)	F_c^{exp} (N)	F_c^{sim} (N)	Err. (%)	F_p^{exp} (N)	F_p^{sim} (N)	Err. (%)	T_{TF1}^{exp} (°C)	T_{TF1}^{sim} (°C)	Err. (%)	$T_{\text{max}}^{\text{sim}}$ (°C)	$z_{gs < 1}^{\text{exp}}$ (μm)	$z_{gs < 1}^{\text{sim}}$ (μm)	Err. (%)
50	890	915	2.8	210	225	7.1	122	130	6.6	612	2.4	2.3	4.2
150	760	780	2.6	185	195	5.4	168	175	4.2	715	1.6	1.7	6.3
250	670	650	3.0	162	157	3.1	203	210	3.4	816	3.7	3.6	2.7

Table 6.2: Validation for $VB = 150 \mu\text{m}$: predicted vs. measured forces, TF1 temperature, and UFG layer thickness. Relative error = $|Sim - Exp|/Exp \times 100\%$. T_{max} is simulation-only.

v_c (m/min)	F_c^{exp} (N)	F_c^{sim} (N)	Err. (%)	F_p^{exp} (N)	F_p^{sim} (N)	Err. (%)	$T_{\text{TF1}}^{\text{exp}}$ (°C)	$T_{\text{TF1}}^{\text{sim}}$ (°C)	Err. (%)	$T_{\text{max}}^{\text{sim}}$ (°C)	$z_{\text{gs}<1}^{\text{exp}}$ (μm)	$z_{\text{gs}<1}^{\text{sim}}$ (μm)	Err. (%)
50	930	955	2.7	255	270	5.9	138	146	5.8	645	2.9	2.8	3.4
150	800	820	2.5	225	238	5.8	180	188	4.4	752	2.0	2.1	5.0
250	700	685	2.1	200	210	5.0	215	224	4.2	840	4.1	4.0	2.4

Table 6.3: Validation for $VB = 300 \mu\text{m}$: predicted vs. measured forces, TF1 temperature, and UFG layer thickness. Relative error = $|Sim - Exp|/Exp \times 100\%$. T_{max} is simulation-only.

v_c (m/min)	F_c^{exp} (N)	F_c^{sim} (N)	Err. (%)	F_p^{exp} (N)	F_p^{sim} (N)	Err. (%)	$T_{\text{TF1}}^{\text{exp}}$ (°C)	$T_{\text{TF1}}^{\text{sim}}$ (°C)	Err. (%)	$T_{\text{max}}^{\text{sim}}$ (°C)	$z_{\text{gs}<1}^{\text{exp}}$ (μm)	$z_{\text{gs}<1}^{\text{sim}}$ (μm)	Err. (%)
50	980	1005	2.6	385	400	3.9	152	161	5.9	690	3.3	3.2	3.0
150	840	865	3.0	260	275	5.8	190	200	5.3	785	2.9	3.0	3.4
250	730	715	2.1	260	270	3.8	225	235	4.4	860	4.6	4.5	2.2

6.2.4 Simulated Process Maps

The 3D FEM simulations provide a high-fidelity dataset that enables the construction of two-dimensional process maps over the (v_c, a_p) domain for unworn and worn tools. These maps summarise the evolution of cutting forces, thermal fields, and microstructural refinement, and offer a compact yet physically meaningful representation of the parameter space.

The maps shown in Figs. 6.7–6.8 were generated from the DOE grid ($v_c \in \{50, 150, 250\}$ m/min, $a_p \in \{0.3, 0.6, 1.2\}$ mm) using second-order polynomial surface interpolation. This choice ensures physically smooth fields while avoiding oscillations associated with higher-order fits. No extrapolation beyond the convex hull of the DOE points was performed; thus, the maps represent strictly interpolated simulation outcomes.

The quantities visualised are: tangential force (F_c), feed force (F_f), passive force (F_p), the measured-tool temperature (T_{TF1}), the surface flash temperature (T_{max}), and the UFG layer thickness $z_{\text{gs}<1 \mu\text{m}}$. All maps use identical colour scales across wear states, enabling direct comparison between the unworn ($VB = 0 \mu\text{m}$) and severely worn ($VB = 300 \mu\text{m}$) cases.

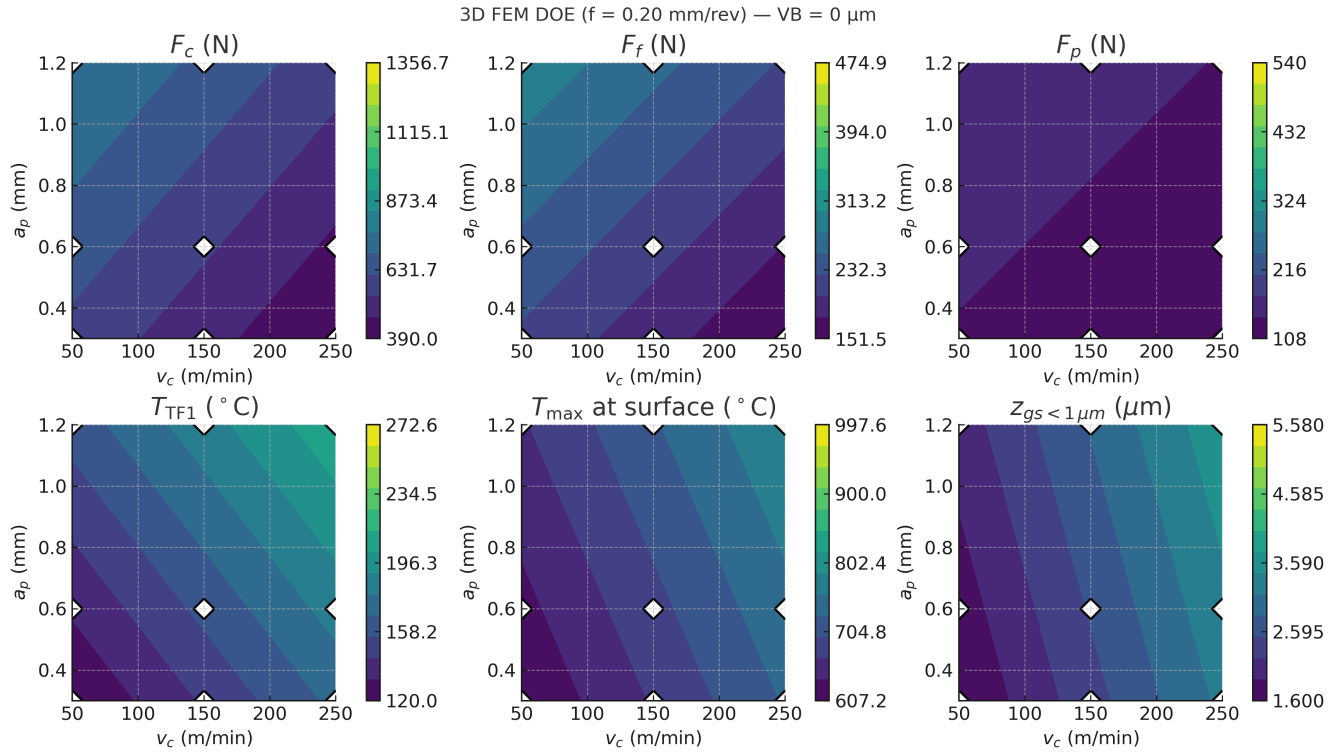


Figure 6.7: 3D FEM process maps at $f = 0.20$ mm/rev for $VB = 0$ μm . Diamond markers indicate DOE nodes ($v_c = 50, 150, 250$ m/min; $a_p = 0.3, 0.6, 1.2$ mm).

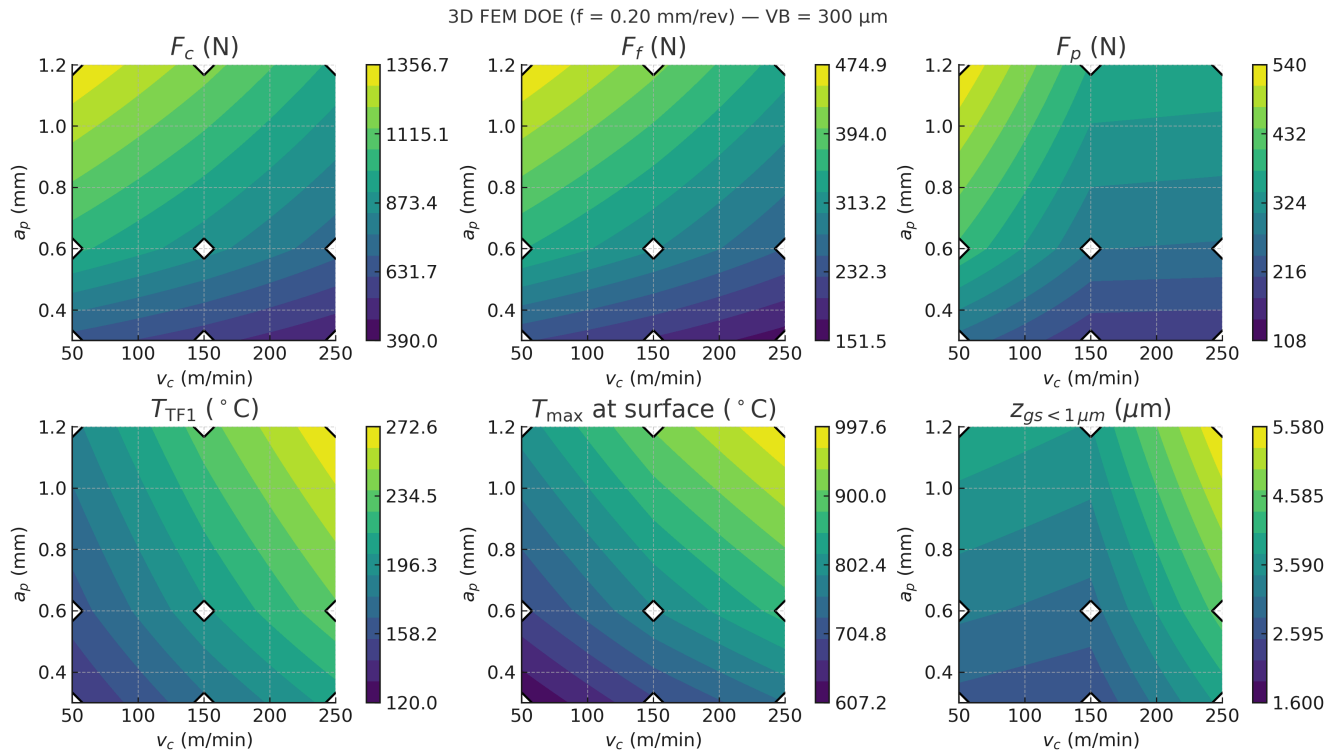


Figure 6.8: 3D FEM DOE process maps at $f = 0.20$ mm/rev for $VB = 300$ μm . Identical colour scales allow direct comparison to Fig. 6.7.

Scaling effect of cutting forces: For both wear states, F_c and F_f increase nearly linearly with a_p and exhibit only weak dependence on v_c . This behaviour mirrors the area-proportional scaling of the undeformed chip thickness and is consistent with the experimental force trends presented in Fig. 6.1.

The weak v_c dependence originates from moderate thermal softening and the short contact time of the chip, which limits the influence of cutting speed on the effective flow stress. The corresponding maps (top row in Figs. 6.7–6.8) exhibit nearly planar surfaces, indicating that F_c and F_f are dictated primarily by chip load.

Thermo-mechanical fields: The temperature maps show a much stronger dependence on both cutting speed and depth of cut. T_{TF1} increases monotonically with v_c and a_p , reflecting the higher shear energy input at elevated cutting speeds and the longer tool–chip contact length at larger engagements. The surface flash temperature T_{max} behaves similarly but with significantly steeper gradients, especially at high a_p . This sensitivity originates from the localised nature of heat generation in the primary shear zone and the rapid heat dissipation into the tool.

In worn tools, both T_{TF1} and T_{max} are noticeably higher. The wear land increases the real contact area between chip and flank, enhancing frictional heat generation and reducing thermal escape routes along the rake face. As a result, the thermal maps for $VB = 300 \mu\text{m}$ shift upward and become more steeply inclined in the high- a_p region.

Wear-sensitive mechanics: The process maps highlight the dominant role of F_p as a wear indicator. Whereas F_c and F_f exhibit similar surfaces for worn and unworn tools, the F_p maps undergo a drastic transformation. For $VB = 0 \mu\text{m}$, F_p increases moderately with a_p and only weakly with v_c . For $VB = 300 \mu\text{m}$, the entire surface shifts upward by more than 100 N, and strong curvature appears in the high- v_c /high- a_p region. This curvature corresponds to an intensified ploughing effect caused by the enlarged wear land and increased normal loading. These features align closely with the experimental wear progression in Fig. 6.3, where F_p rises steeply beyond $VB \approx 150 \mu\text{m}$.

Surface integrity and UFG layer thickness: The maps for $z_{gs} < 1 \mu\text{m}$ provide a unified view of how thermal and mechanical loads jointly govern surface refinement. For the unworn tool, UFG thickness increases with both v_c and a_p , following the growth of strain and temperature in the near-surface region. The strongest sensitivity occurs in the high- a_p domain, where mechanical work input is greatest. In the worn-tool case, the UFG layer thickens dramatically,

especially at high v_c . The wear land causes (i) a shift of the deformation zone deeper into the workpiece, (ii) increased thermal exposure due to additional frictional heating, and (iii) prolonged contact between the tool flank and the freshly generated surface.

These effects combine to produce the elevated UFG levels observed experimentally, presented in Fig. 6.4. Notably, the regions of maximum UFG thickness spatially coincide with regions of elevated F_p and $T_{\max}$, reflecting the linked thermo-mechanical origin of microstructural refinement. Figures 6.7–6.8 illustrate these maps for unworn and worn tools using consistent colour limits for direct visual comparison.

All trends in the maps are consistent with the experimental measurements presented in Chapter 6. In particular, the strong sensitivity of F_p and UFG layer thickness to wear, as well as the monotonic increase of T_{TF1} with cutting speed, agree with the experimental data. The correspondence between simulation-derived UFG thickness and SEM-based measurements further confirms that the maps capture both the thermo-mechanically driven surface modification and its dependence on process parameters. The process maps reveal regions where thermal and mechanical loads reach levels that may lead to undesirable surface modification or accelerated wear. Combinations of high a_p and high v_c produce the largest values of $T_{\max}$ and F_p , which are associated with surface degradation and rapid wear progression. Conversely, lower v_c and moderate a_p provide favourable conditions with reduced UFG thickness and lower forces, offering a practical operating window for minimising wear and preserving surface integrity. Because the maps encode the deterministic relationship between machining parameters, wear state, and thermo-mechanical fields, they form the basis for the Bayesian inference framework developed in the next chapter. Thus, the process maps not only summarise the simulation results but also serve as a forward model for rapid, wear-dependent surface-integrity prediction within the subsequent Bayesian framework.

6.2.5 Model Limitations and Uncertainty

Although the 3D FEM framework reproduces forces, temperatures, and surface grain refinement with high accuracy, several sources of modelling uncertainty remain and should be considered when interpreting the results. The first concerns mesh sensitivity. Small variations in element size in this region can influence the peak thermal and mechanical gradients that drive DRX activation.

A second source of uncertainty arises from the friction model. The Coulomb–viscous formulation, while widely used in machining simulations, cannot fully represent the complex evolution of frictional behaviour under worn-tool conditions. Adhesion, changing real contact area, and

ploughing effects modify the local friction state during cutting, and the corresponding variations in normal stress are only approximately reproduced by a fixed friction coefficient. As a consequence, predictions of F_p under severe wear may exhibit small systematic deviations.

The representation of tool wear introduces an additional limitation. The wear lands used in the simulations are idealised geometries that were prescribed a priori, whereas real tools may exhibit asymmetric flank wear, crater wear on the rake face, micro-chipping, or localised edge damage. These forms of wear change heat partition, contact mechanics, and chip flow in ways that are not captured by the present parametrised approach. Although the idealised wear geometries reproduce the dominant trends in F_p and surface integrity, they cannot account for all wear-induced effects observed in practice.

A fourth limitation concerns the treatment of microstructure. The dislocation-density-based DRX model is applied in post-processing and does not affect the constitutive response of the material. Consequently, neither recrystallisation-induced softening, associated with dislocation annihilation and dynamic recovery, nor strain-induced hardening resulting from severe plastic deformation feeds back into the flow stress. The mechanical response is therefore governed exclusively by the calibrated Johnson–Cook law, while the predicted microstructural state reflects a one-way coupling from the thermomechanical fields to grain refinement. As a result, the simulated forces and temperatures remain unaffected by microstructural evolution, and the predicted grain sizes should be interpreted as kinematic outcomes of the deformation history rather than as drivers of the constitutive behaviour.

6.3 Discussion

The combined experimental and numerical analyses presented establish a robust and internally consistent link between cutting parameters, flank wear progression, thermo-mechanical loading, and surface integrity. The relationship is governed primarily by the evolution of contact conditions at the flank face, which controls both the mechanical load on the tool and the deformation history imposed on the near-surface material. While the tangential and feed forces (F_c and F_f) exhibit only moderate increases with growing wear land, F_p responds nonlinearly once VB exceeds approximately $150\ \mu\text{m}$. This rapid increase reflects the enlargement of the tool–workpiece contact area and the corresponding rise in normal stress and ploughing resistance in the tertiary deformation zone. The behaviour is mirrored directly in the microstructural response: the thickness of the ultrafine-grained (UFG) layer $z_{\text{gs}<1\ \mu\text{m}}$ increases by roughly 100–150% between the unworn and heavily worn conditions. The close correspondence between F_p and z_{gs} across all cutting speeds provides strong evidence that the passive force offers the clearest in-process signature of wear-induced surface modification.

The results further clarify the respective roles of mechanical deformation and thermal exposure in driving microstructural refinement. Although both T_{TF1} and the simulated surface flash temperature T_{max} increase systematically with cutting speed and wear level, no white layers were observed experimentally. This absence implies that surface modification in this process window is not thermally dominated. Rather, the microstructural refinement is governed primarily by severe plastic deformation and dynamic recrystallisation. Thermal softening enhances the kinetics of DRX but does not fundamentally change the mechanism, indicating that refinement arises from a mechanically dominated process with temperature acting mainly as an accelerator.

The predictive performance of the 3D FEM framework reinforces this mechanistic interpretation. The model reproduces cutting forces, tool-side temperatures, and UFG layer thicknesses with typical errors of 5–7% across all wear states. This level of accuracy confirms the benefit of resolving flank contact mechanics, spatially distributed heat conduction, and the three-dimensional strain field—features that cannot be captured in a 2D formulation. At the same time, the analysis highlights two methodological limitations: the absence of two-way coupling between microstructure and constitutive behaviour, and the use of prescribed wear geometries rather than a progressive wear-growth law. These limitations do not compromise the validity of the main trends, but they restrict the model's ability to predict the temporal evolution of wear during cutting.

Taken together, the results demonstrate that the 3D FEM framework offers a quantitatively reliable basis for predicting machining-induced microstructure and surface integrity across a wide range of cutting conditions and wear states. They also point toward the need for models that integrate wear progression directly into the simulation environment. This motivates the development of the Bayesian wear-inference framework introduced in the subsequent chapter, which enables probabilistic estimation of the instantaneous wear state and provides the necessary link between progressive tool degradation and surface integrity prediction.

7 Results of Bayesian Tool-Wear Modelling

This chapter presents the application of the Bayesian inference framework introduced in Section 4.7 to the prediction of flank-wear progression in longitudinal turning and its integration with the 3D FEM surface integrity results. In contrast to deterministic regression, which yields a single best-fit curve for tool wear, the Bayesian formulation provides full posterior distributions for the wear model parameters and for the wear trajectory itself. These posteriors quantify uncertainty, allow prior knowledge to be transferred between cutting conditions, and enable sequential updating as new measurements become available. The exponential degradation model used here has already been introduced and justified in Section 4.7 as a classical state-of-the-art representation of tool wear. The focus in this chapter is therefore not on model formulation, but on inference quality, information transfer across cutting speeds, and the propagation of wear uncertainty into FEM-based predictions of forces, temperatures, and microstructural refinement.

7.1 Conventional Deterministic Approach

As a baseline, flank wear $VB(t)$ was first modelled with a conventional nonlinear least-squares fit of the exponential degradation law defined in Eq. 4.44. This provides a single deterministic parameter pair (a, b) that best reproduces the measured wear curve in a least-squares sense. Figure 7.1 shows the result for MP6 inserts at $a_p = 1.5$ mm, $f = 0.15$ mm/rev, and $v_c = 200$ m/min. When all available data points are used for calibration, the exponential model reproduces the experimental wear progression very well, with fitted parameters $a \approx 0.0973$, $b \approx 0.0218$ and a coefficient of determination $R^2 = 0.992$.

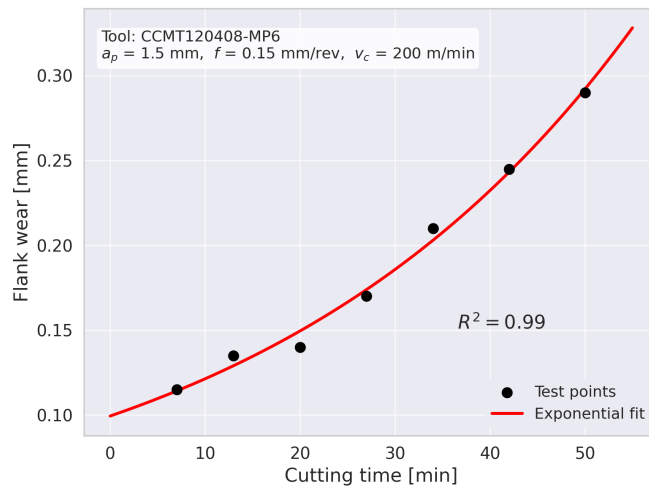


Figure 7.1: Nonlinear least-squares exponential fit of flank wear at $v_c = 200$ m/min using the full dataset.

Under such data-rich conditions, the exponential law captures the main features of the wear evolution, including its accelerating nature in the later stages of tool life. However, the limitations of the deterministic approach become evident as soon as the calibration is restricted to early-life data.

Figure 7.2 illustrates this behaviour for $v_c = 250$ m/min, where only the first five measurements (up to 18 min of cutting time) are used for fitting. While the regression reproduces the initial, slowly increasing wear segment, it fails to anticipate the subsequent acceleration of VB . When the fitted curve is evaluated against the complete dataset, the coefficient of determination drops to $R^2 = 0.13$. This represents a qualitatively incorrect extrapolation: depending on the threshold used, the model may either severely underestimate tool life or dangerously overestimate it. The example highlights that purely deterministic regression is not sufficient for early-stage prediction, as it provides neither uncertainty quantification nor a mechanism to include prior knowledge from previous tests.

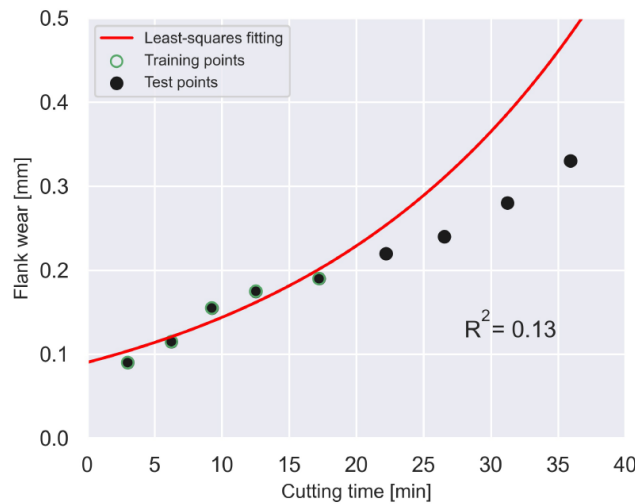


Figure 7.2: Exponential wear growth using nonlinear least-squares fit at $v_c = 250$ m/min. Only the first five data points (up to 18 min) were used for calibration; model quality was assessed on the full dataset.

7.2 Bayesian Inference for Wear Evolution

The same exponential model is now embedded in the Bayesian framework described in Section 4.7. Flank wear VB_i observed at time t_i is represented as

$$VB_i = b \exp(at_i) + \varepsilon_i, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma_{VB}^2), \quad 7.1$$

with a the wear-growth rate, b the initial wear level, and σ_{VB} the standard deviation of the measurement noise. Weakly informative priors are assigned according to Section 4.7, and the posterior $p(a, b, \sigma_{VB} \mid VB_{1:n})$ is obtained via Hamiltonian Monte Carlo using the No-U-Turn

Sampler (NUTS). The diagnostics consistently satisfy $\hat{R} < 1.01$ and large effective sample sizes, indicating reliable exploration of the posterior.

For the dataset at $v_c = 200$ m/min, the uniform priors on a and b over $[0, 0.2]$ contract strongly once the data are assimilated. Figure 7.3 compares the prior and posterior distributions for a and b . The posterior mean and standard deviation for a are approximately 0.091 and 0.006, respectively, while b is identified with a posterior mean near 0.023 and a standard deviation of about 0.002. The substantial reduction in spread relative to the priors demonstrates that the available wear measurements at $v_c = 200$ m/min are informative and lead to a well-identified exponential growth law.

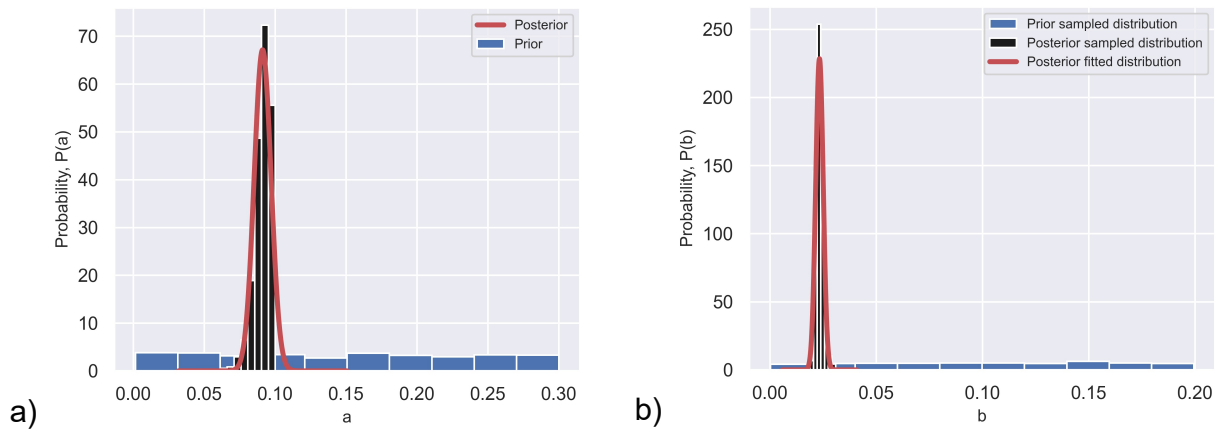


Figure 7.3: Prior and posterior distributions for parameters a and b at $v_c = 200$ m/min. The posteriors show strong contraction relative to the weakly informative uniform priors.

The corresponding posterior predictive distribution for the wear trajectory is shown in Fig. 7.4. The posterior mean closely follows the measured data, and the pointwise $\pm 1\sigma$ credible band encloses all experimental points.

The predictive R^2 value of 0.98 is consistent with the deterministic fit, but in contrast to the latter, the Bayesian approach delivers a full uncertainty envelope rather than a single curve. Defining tool life T^* as the first time at which $VB(T^*) = VB_{\text{crit}}$ with $VB_{\text{crit}} = 0.29$ mm, the posterior samples of (a, b) yield a distribution of T^* rather than a single value. The median of this distribution is approximately 49.8 min, and credible intervals follow directly from the posterior samples, expressing the probability that the tool reaches the critical wear level before or after a given cutting time.

Sequential updating and transfer of information between cutting speeds

A central advantage of the Bayesian formulation is its ability to reuse information acquired in previous experiments. In the present context, the posterior determined for $v_c = 200$ m/min is

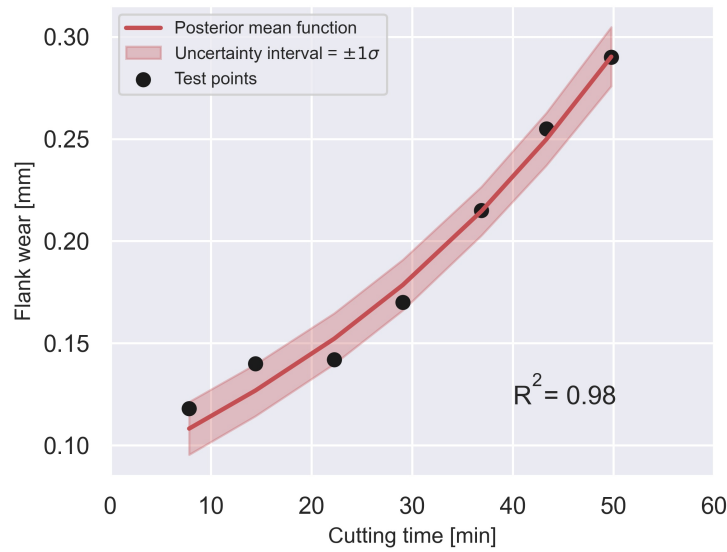


Figure 7.4: Bayesian prediction of flank wear at $v_c = 200$ m/min: posterior mean and pointwise $\pm 1\sigma$ band, together with the experimental data used for calibration and validation.

used as an informative prior for the subsequent experiment at $v_c = 250$ m/min. Physically, the underlying wear mechanisms (abrasion, adhesion, oxidation) remain the same, but the higher cutting speed intensifies the thermo-mechanical loading and is expected to increase the wear-growth rate. The informative prior is therefore centred at the $v_c = 200$ m/min posterior means, but its variance is retained or slightly inflated to avoid over-constraining the new inference.

Calibration at $v_c = 250$ m/min is then carried out using only the first five wear measurements (up to 18 min). Figure 7.5 shows the resulting posterior predictive mean and $\pm 1\sigma$ credible band. Despite using extremely limited calibration data, the predictive curve tracks the full wear evolution with high accuracy, achieving $R^2 = 0.96$ when compared to the complete dataset. In particular, the exponential acceleration in the later stages is captured, in severe contrast to the deterministic least-squares fit trained on the same early points (Fig. 7.2). The difference arises because the Bayesian model leverages prior knowledge of the wear kinetics, while still allowing the data at $v_c = 250$ m/min to adjust the parameters.

To test generalisation across operating regimes, a similar strategy is applied in the opposite direction. The posterior from $v_c = 200$ m/min is used to construct a prior for a new experiment at the lower cutting speed $v_c = 100$ m/min. In this case, the wear growth rate a is expected to be smaller due to the reduced sliding speed and thermal load. The prior for a is therefore centred at the $v_c = 200$ posterior mean but widened to reflect the reduced driving forces. After updating with the available measurements at $v_c = 100$ m/min, the posterior yields the predictive mean and credible band shown in Fig. 7.6. The predicted curve tracks the measured

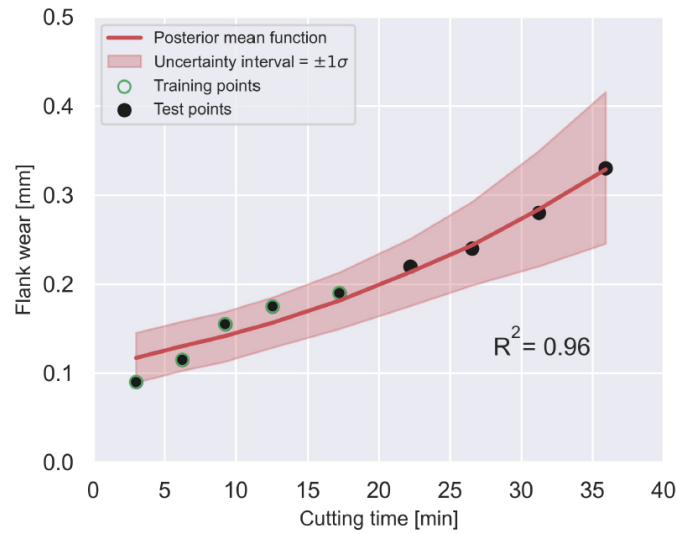


Figure 7.5: Bayesian tool-wear prediction at $v_c = 250$ m/min using informative priors obtained from the $v_c = 200$ m/min experiment and only the first five measurements for updating.

wear data well over the full cutting horizon, confirming that informative priors learned at one cutting speed can be transferred to neighbouring regimes without loss of consistency.

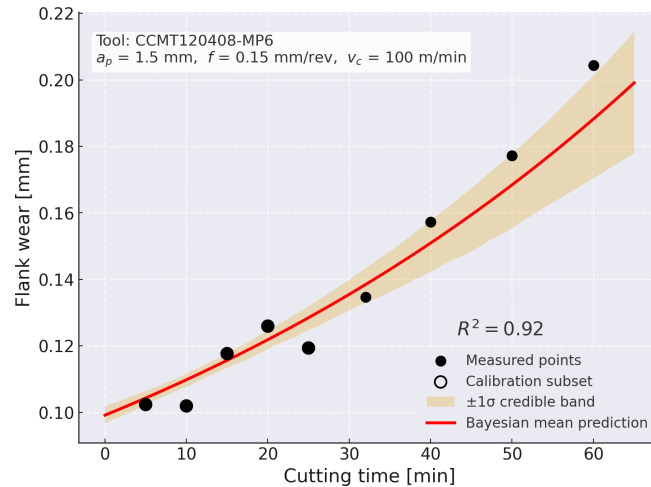


Figure 7.6: Bayesian tool-wear prediction at the lower cutting speed $v_c = 100$ m/min using informative, variance-widened priors transferred from the $v_c = 200$ m/min experiment.

Posterior predictive checks for all speeds show no systematic structure in the residuals, and the empirical coverage of the credible bands is close to the nominal levels, indicating that the uncertainty quantification is well calibrated. Comparisons with alternative functional forms (quadratic or Gompertz-type models) confirm that, within the present parameter window, the exponential law provides the most robust extrapolation behaviour, particularly when combined with prior information.

7.3 Bayesian–FEM Coupling for Surface-Integrity Prediction

The Bayesian wear model introduced in Section 4.7 is designed to interface directly with the 3D FEM database developed in Chapter 6. The posterior distribution of the wear-law parameters (a, b) induces a distribution of wear states $VB(t)$, where each state corresponds to one of the discrete tool geometries used in the simulations (e.g. $VB = 0, 150$, and $300 \mu\text{m}$). Mapping posterior samples of $VB(t)$ onto the FEM results enables the propagation of uncertainty in the inferred wear state into uncertainty in forces, temperatures and microstructural indicators.

The FEM validation tables (Tables 6.1, 6.2 and 6.3) provide a deterministic mapping from wear level to process response for each cutting speed. For example, at $v_c = 250 \text{ m/min}$ the UFG-layer thickness increases from approximately $3.7 \mu\text{m}$ at $VB = 0 \mu\text{m}$ to $4.1 \mu\text{m}$ at $VB = 150 \mu\text{m}$ and $4.6 \mu\text{m}$ at $VB = 300 \mu\text{m}$, while the flash temperature $T_{\max}$ rises from about 816°C to 840°C and 860°C over the same interval. Across all cutting speeds, the FEM database therefore establishes a deterministic mapping

$$VB \longrightarrow (F_c, F_p, T_{\text{TF1}}, T_{\max}, z_{\text{gs}<1}).$$

Embedding this mapping into the Bayesian framework converts it into a probabilistic one. For a given cutting time t , each posterior sample $(a^{(k)}, b^{(k)})$ produces a wear state

$$VB^{(k)}(t) = b^{(k)} \exp(a^{(k)}t),$$

which is then assigned to the nearest available FEM wear level or interpolated between adjacent levels. This produces an ensemble of predictions

$$\{F_p^{(k)}(t), T_{\max}^{(k)}(t), z_{\text{gs}<1}^{(k)}(t)\}_{k=1}^N,$$

representing uncertainty-aware estimates of passive force, flash temperature and UFG-layer thickness at time t . In this sense, uncertainty in $VB(t)$ inferred from limited measurements is consistently propagated through the FEM-based process model.

The mechanism is illustrated for $v_c = 250 \text{ m/min}$. If the posterior for $VB(t)$ places substantial probability mass between 150 and $300 \mu\text{m}$, then samples near the lower bound map to microstructures with $z_{\text{gs}<1}$ close to $4.1 \mu\text{m}$, whereas samples near $300 \mu\text{m}$ yield values around $4.6 \mu\text{m}$. The resulting predictive distribution of $z_{\text{gs}<1}(t)$ reflects both the strong sensitivity of the microstructure to wear progression and the uncertainty in the inferred wear state. Analogous behaviour is observed for F_p and $T_{\max}$, which also exhibit nonlinear increases with wear. This Bayesian–FEM coupling extends the deterministic simulation framework into an

uncertainty-resolved prediction tool. Instead of single-point estimates, the approach yields credible intervals for microstructural depth, flash temperature or passive force at any given cutting time. From a process-design perspective, this enables risk-informed statements such as the probability that the UFG-layer thickness exceeds a functional threshold within a given monitoring horizon or that $T_{\max}$ enters a critical regime under a proposed parameter set. The integration of Bayesian wear inference with the FEM database thus provides a coherent, uncertainty-aware basis for predictive surface-integrity engineering.

7.4 Soft-Sensor for Uncertainty-Aware Surface-Integrity Prediction

Building upon the regression framework and the Bayesian tool-wear inference described in the previous sections, the present work integrates these components into a hybrid *soft-sensor* architecture for predictive surface-integrity monitoring. As introduced conceptually in Section 4.8, the soft sensor combines high-fidelity FEM simulations, data-driven surrogate modelling and probabilistic wear estimation to reconstruct microstructural quantities that are not directly measurable during machining. The soft sensor operates along two complementary pathways. The *offline pathway* is driven by the calibrated 2D and 3D FE models, which together generate a high-resolution database of thermomechanical fields and microstructural outputs across a full factorial range of cutting speeds, feeds and tool-wear levels. Regression-based surrogate models trained on this database allow the grain-size response to be interpolated rapidly over the continuous process window. This enables offline process planning and sensitivity analysis, where the influence of cutting parameters and wear state on surface integrity can be evaluated without rerunning computationally expensive FE simulations.

The *sequential-update pathway* augments these offline predictions by incorporating newly available information about the evolving tool-wear state. Since direct measurement of flank wear is typically unavailable during machining, the Bayesian degradation model introduced previously is used to infer wear from cutting time and, when available, sparse wear observations. The resulting posterior distribution provides not only a wear estimate but also its associated uncertainty. This posterior is propagated through the surrogate regression model to obtain updated grain-size predictions that reflect the current tool condition. When additional measurements are recorded, the posterior is recursively updated by re-running MCMC with the previous posterior as the new prior, enabling sequential refinement of both the wear estimate and the corresponding surface-integrity predictions.

The hybrid structure of the soft sensor therefore mirrors the modelling workflow introduced earlier (Fig. 4.26), where the deterministic surrogate models represent the computational core and the Bayesian module provides sequential, uncertainty-aware updating. In combination, these elements support *offline surface-integrity prediction* for process planning and establish

the methodological basis for process-accompanying predictive monitoring and future closed-loop control.

7.5 Discussion

The Bayesian modelling of tool wear developed in this chapter complements the deterministic 3D FEM simulations of Chapter 6 by adding a rigorous layer of uncertainty quantification and adaptive learning. When detailed wear data are available, the Bayesian model converges to results that are essentially indistinguishable from nonlinear least-squares fits, but with the important addition of credible intervals for both the wear trajectory and the derived tool-life metrics. When only early-life measurements are available, deterministic regression shows pronounced limitations, particularly at higher cutting speeds where the later acceleration in wear is not yet visible. In these cases, the Bayesian approach demonstrates a clear advantage: by carrying forward information from previously observed cutting conditions in the form of informative priors, it delivers predictive curves and tool-life estimates that remain consistent with the eventual evolution of wear.

Beyond predicting $VB(t)$ itself, the main added value of the Bayesian framework lies in its integration with the FEM-based description of process forces, temperatures, and surface integrity. The 3D FEM database provides a mapping between discrete wear states and metrics such as passive force and UFG layer thickness. By feeding posterior samples of $VB(t)$ through this mapping, uncertainty in the inferred wear state is translated into uncertainty in surface integrity. The results confirm trends already identified experimentally and numerically in the previous chapters: F_p and $z_{gs<1}$ are particularly sensitive to wear progression and exhibit nonlinear growth beyond $VB \approx 150 \mu\text{m}$, while T_{max} increases with both cutting speed and wear but remains below the level required for extensive white-layer formation under the tested conditions. The Bayesian–FEM coupling therefore provides a coherent picture in which flank wear controls both the magnitude of passive forces and the depth of mechanically and thermally driven surface refinement.

From an operational perspective, the availability of posterior distributions for $VB(t)$ and surface integrity metrics supports risk-aware decision making. Tool-change times can be defined not only by a deterministic estimate of when VB reaches a critical value, but also by specifying an acceptable probability that $VB(\tau)$ or $z_{gs<1}(\tau)$ exceed their functional limits at a prospective change time τ . This probabilistic framing aligns well with the intrinsic variability of machining processes and with industrial needs for robust, rather than purely nominal, process windows.

8 Overall Conclusions

This thesis establishes an integrated experimental–computational framework for predicting wear-dependent surface integrity in hard turning. The central hypothesis was that a physics-based, microstructure-aware process model, informed by tool-integrated sensing and augmented with probabilistic inference, could provide more reliable and informative predictions of surface-state evolution than conventional deterministic modelling alone. The research objectives were therefore to develop a finite-element representation of chip formation capable of reproducing the thermomechanical fields relevant to dynamic recrystallisation and grain refinement; to design and integrate thin-film sensors for co-located temperature and wear-related measurements; to formulate a Bayesian inference approach for early and uncertainty-aware estimation of flank-wear progression; and to unify these components within an open-loop soft-sensor architecture for predicting the microstructural condition of the machined surface, thereby providing a basis for future in-process deployment.

These objectives were addressed through a sequence of closely coupled methodological developments. A 2D FE model was first calibrated against controlled orthogonal-cutting experiments using synchronised force measurements, high-resolution temperature sensing and post-process microstructural analysis. The flow-stress, friction and DRX formulations were calibrated to reproduce the measured thermomechanical and microstructural responses. Building on this foundation, the model was extended to 3D turning configurations, providing spatially resolved thermomechanical fields and DRX-based metrics across a matrix of cutting speeds, feeds and wear states. The 3D simulations were validated against dedicated turning experiments and subsequently used to construct an FE database from which surrogate regression models were trained. These surrogates enable rapid interpolation of microstructural responses without rerunning the computationally expensive FE simulations. In parallel, thin-film thermistors and resistive wear tracks were fabricated directly on industrial cutting inserts, enabling time-aligned acquisition of temperature and wear-related signals under machining conditions relevant to industrial practice.

Across the investigated cutting conditions, the experimental and numerical results consistently showed that progressive flank wear intensifies the thermomechanical loading of the newly generated surface. In particular, passive force, flash temperature and ultrafine-grained layer depth increased with tool wear, with passive force and UFG-layer thickness exhibiting particularly strong wear sensitivity. The agreement between measured and simulated forces, temperatures and near-surface microstructures supports the use of the calibrated FE database as a physically grounded forward model for wear-dependent surface-integrity prediction.

A central contribution of the thesis is the Bayesian formulation of flank-wear evolution. By embedding an exponential wear law within a probabilistic framework and performing inference using Markov chain Monte Carlo sampling, wear progression can be estimated from sparse observations together with credible intervals that express parameter and measurement uncertainty. Information obtained at one cutting speed can be transferred to neighbouring conditions through informative priors, enabling early-stage prediction when only a limited portion of the wear curve has been observed. The resulting posterior distributions describe both the wear-law parameters and the corresponding wear trajectory, providing point estimates together with uncertainty bounds.

Samples drawn from these posterior distributions serve as stochastic inputs to the surrogate models and, by extension, to the microstructure predictions derived from the FE database. In this way, uncertainty in the estimated wear state is propagated consistently through the modelling chain and into surface-integrity metrics such as UFG-layer thickness, passive force and flash temperature. The Bayesian–FEM coupling therefore extends the deterministic simulation framework from single-value predictions to uncertainty-resolved estimates that can support risk-aware process assessment.

The soft-sensor architecture developed in this thesis integrates these components within a hybrid open-loop framework for offline prediction and sequential updating. In the offline pathway, the calibrated FE simulations and regression surrogates form a process map linking cutting parameters and tool wear to thermomechanical loading and microstructural refinement. In the sequential-update pathway, the Bayesian inference layer incorporates newly available wear observations and updates the posterior distribution of the wear-law parameters and the induced wear state $VB(t)$. This updated distribution is subsequently propagated through the surrogate layer to yield uncertainty-aware estimates of the current and projected surface state.

The combination of physics-based modelling, data-driven interpolation and probabilistic inference transforms heterogeneous information into a coherent basis for decision support. Evaluation of the surrogate models is computationally inexpensive compared with rerunning the complete FE model and therefore offers potential for future execution alongside machine tools. Following real-time integration and on-machine validation, the framework could provide in-process indicators of surface integrity and remaining useful life relative to predefined surface-quality limits.

The scientific significance of the work lies in establishing a mechanism-consistent pathway linking chip-formation physics, tool wear and surface integrity within a single uncertainty-aware framework. Coupling FE-derived microstructure metrics with Bayesian wear inference

represents a methodological advance over conventional deterministic surface-prediction models, which generally provide single-point estimates without explicit uncertainty quantification. The integration of sensor data further strengthens the physical basis of the framework by providing independent tool-tip temperature measurements and wear-related observations for model calibration and validation. More broadly, the thesis demonstrates how sensor-informed, microstructure-aware physics can be incorporated into probabilistic digital models that provide a foundation for process planning, monitoring and future control.

Despite these contributions, several limitations remain. The microstructure model is one-way coupled and does not feed back into the flow-stress or friction formulations of the FE model. Grain growth and post-cut recrystallisation, which may become relevant for other materials or thermal cycles, are not included. The Bayesian wear model employs a single exponential degradation law with homoscedastic noise and therefore does not yet account for between-tool variability, batch-to-batch effects or heteroscedastic measurement uncertainty. In addition, the surrogate models are reliable only within the parameter domain represented by the FE database. Adaptive sampling, uncertainty-aware regression or explicit out-of-domain detection would therefore be required to reduce the risk of unreliable extrapolation.

Finally, the soft sensor has been demonstrated in an offline, open-loop configuration. Its integration into closed-loop control requires additional real-time sensing, automated data transfer, bounded-latency inference, runtime validation and on-machine demonstration.

Future research should therefore focus on embedding microstructure evolution directly within the constitutive description of the FE model, thereby enabling two-way coupling between local microstructural state variables and thermomechanical fields. State-dependent friction and heat-partition formulations, together with coolant and lubrication effects, should be incorporated to improve predictive accuracy under industrial machining conditions. Hierarchical Bayesian models could account for variability across individual tools, geometries, material batches and cutting conditions, enabling population-level inference rather than tool-specific calibration.

From a digitalisation perspective, uncertainty propagation should be extended across the complete sensing, inference, physics and decision chain. The next major step is an on-machine closed-loop demonstrator in which in-process measurements are used to update the estimated wear state sequentially and the resulting surface-integrity predictions are used to adjust cutting parameters under validated process and quality constraints.

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