50 years of nanomechanics: Scale-bridging mechanistic insights through the looking glass

Seung Min Han,* Daniel S. Gianola, Carlos M. Portela, Marco Sebastiani, and Christoph Kirchlechner

Historical and recent advances in the field of nanomechanics, ranging from the early development of nanoindentation to recent advances in artificial intelligence- and machine learning-based characterization and modeling are covered in this article. Early advances were motivated by thin-film mechanics challenges driven by the microelectronics industry. In the ensuing years, different methodologies for probing mechanical properties at length scales relevant to a myriad of applications and materials systems have been developed, coupled with a variety of *in situ* testing methods that shed insights into new mechanisms. Built upon the knowledge base from nanomechanics, new mechanical metamaterials with otherwise unachievable material properties have been discovered, and new methods in testing and analyzing properties for extreme conditions have been recently reported. This article discusses the journey that the nanomechanics community has gone through over the past 50 years and shares the scale-bridging mechanistic insights through the looking glass.

Introduction

The field of nanomechanics has advanced significantly over the past 50 years. As the microelectronics industry continued to miniaturize technologies that involve smaller-scale structures with an increase in structural complexity, the understanding of mechanical properties and stress evolution in multilayered thin-film structures to ensure device reliability has been actively researched since the 1980s. Thin films are reported to have wildly different mechanical properties in comparison to the bulk, which is now understood to be due to the constraint on dislocations from the substrate, resulting in strength enhancement in thinner films.[1] The key to understanding the length-scale-dependent mechanical properties is in studying how plasticity carriers, such as dislocations, move and interact within constrained small volumes. The development of nanoindentation[2] that later allowed for compression tests of focused ion beam (FIB) milled micro-/nanopillars using the flat punch tip of the nanoindenter,[3] fracture testing,[4] and a variety of *in situ* testing methods accompanied by modeling, has enabled the understanding of nanomechanical behavior at the relevant length scales. New mechanisms that govern mechanical properties at previously unexplored length scales have shaped the understanding of nanomechanics that we know today. Among all of the significant advances in the field, we highlight some of the major developments and scientific discoveries during the past 50 years and call attention to some ongoing current research topics as well as the future direction of nanomechanics.

Nanoindentation and thin-film mechanical properties

The invention of nanoindentation in the 1980s has opened up the door for the field of nanomechanical testing, where one can probe the mechanical properties of materials at the relevant length scales.[2] The Oliver and Pharr (O&P) method published in the *Journal of Materials Research* in 1992[5] is one of the most widely cited articles in the field of materials science, and this points to the importance of the development of the nanoindentation methodology in understanding the mechanical properties of materials. Initial application of the nanoindentation method involved the use of a self-similar Berkovich tip to probe the modulus and hardness of the materials. Continuous measurements of displacement, load, and contact stiffness with the needed fine resolutions suitable for probing micron to

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nanoscale materials, together with contact mechanics, allowed for testing of hardness and modulus of small-scale materials. The O&P method has played a crucial role in the development of modern small-scale mechanical characterization techniques.

With the advances in the microelectronics industry in the late 1980s, there has been a significant technological interest in understanding the thin-film mechanical properties, as severe stress development causes reliability issues such as delamination and fracture in multilayered structures. Although the O&P method is the most widely used method of analysis for nanoindentation, thin film on an elastically mismatched substrate can cause significant pileup or sink-in that limits the accuracy of the O&P method, which was developed for an elastically homogeneous half-space with no pileup or sink-in. Various models have been developed that can remove the substrate effects, such that one can get to the "true" properties of thin films. The Han–Yu–Vlassak method[6] was proposed that can account for the elastic mismatch by incorporating the Yu–Sanday–Rath[7] elastic model to calculate the "true" hardness of a thin film using the stiffness measurements from the continuous stiffness mode (CSM). This has a significant implication, especially on extremely thin films, which would otherwise be dominated by the substrate properties. Determination of thin-film mechanical properties using a nondestructive method is still of urgent technological interest to the microelectronics industry, especially due to the shrinking feature size of integrated circuits. High-κ(high dielectric constant) material thin films with a few nanometers in thickness are already being applied industrially, and advances in thin-film models that allow for the correct determination of extremely thin-layer properties are being researched[8] (see **Figure** 1).

Nanoindentation using a self-similar Berkovich tip imposes an inevitable strain gradient on the samples, and an increase in hardness at small depths known as the indentation size effect has been reported by Nix and Gao[11] to be due to geometrically necessary dislocations (GNDs). The question of whether "smaller is stronger" could not be addressed with sharp tip indentation, but a new method in probing the mechanical properties and deformation mechanisms of small-scale materials was first reported by Uchic et al.,[3] where uniaxial compression tests were performed using a flat punch tip of the nanoindenter to test micropillars fabricated from FIB (**Figure** 2a–b). Clear size-dependent properties were observed in various face-centered-cubic (fcc) metals[3,12] and the different mechanisms were proposed to explain the observed strengthening effect; truncated single-armed dislocation source activation in confined dimensions thus requiring high operation stresses (Figure 2d–e)[13] or dislocation starvation, where dislocations escape to the nearby free surface of nanopillar, requiring higher stress to nucleate new ones (Figure 2f–g).[12,14] Strength increases as the diameter is reduced according to $\sigma \sim D^{-n}$, where the size exponent n is typically around ~0.6 for fcc metals (Figure 2c). For body-centered cubic (bcc) metals with higher Peierls stress, a size dependency was also reported, but with a temperature dependency due to thermal activation over the Peierls barrier.[15,16]

Nanolayered composites with multilayered stacks of thin films have a high density of interfaces and are an example of how thin films with extreme constraints on dislocations can cause ultrahigh strengthening. The strength of multilayers is known to increase with decreasing layer spacing, and such a size effect has been explained by Hall–Petch-type strengthening at submicron scale spacing and by a confined layer slip model at a few tens of nanometers regime (**Figure** 3a).[18] Cu(fcc)-Nb(bcc)-nanolayered composite[19,20] is an example of an incoherent multilayer system, which results in a higher strengthening effect and self-healing of dislocations, which occurs via core-spreading at incoherent interfaces, in comparison to a coherent interface system such as $Al–Al_3Sc$[21] with a continuity in the crystal structure. In both cases, micropillar compression tests revealed that high strengths in the nanolayers can quickly degrade or strain soften as dislocation shears the interfaces, thereby making it less effective in containing dislocations (Figure 3b). To prevent shearing of interfaces, graphene was explored as a mechanism for strengthening the interfaces between metals that showed surprisingly effective strengthening in the metal–graphene nanolayered composites, where the Ni–graphene was reported to be 52% of the theoretical strength of Ni when incorporated with single atomic layer graphene with a layer spacing of 100 nm.[22] Since the first report, there has been extensive research in understanding the deformation mechanisms and also in the development of this material system in the bulk form.

In situ nanomechanical testing: A pathway to multimodal materials characterization

Motivated by the desire to directly observe the dynamic mechanisms underlying elastic and plastic deformation, *in situ* modes of materials testing have vastly expanded over the last 50 years. For instance, directly observing the morphology and kinetics of dislocation dynamics using electron microscopy has enabled a one-to-one correlation between the defect interactions with the lattice or other microstructural features and the extent of mechanical relaxation or strengthening. *Seeing is believing*, as the saying goes.

The more modern eras of *in situ* testing can be loosely chronologized into three periods, as categorized nicely by Legros.[23] The understanding of diffraction conditions that are optimal for imaging defects ushered in a rich first era of elucidating the mechanisms of plasticity, predominantly in structural metals and alloys with technological relevance. For instance, a large portion of our understanding of complex dislocation–precipitate interactions, dislocation dissociations, and faulted structures in superalloys and intermetallics is informed by insights from *in situ* straining in the TEM. Fully instrumented commercial TEM holders were available in the early 2000s that could quantify the deformation and load applied to miniaturized specimens. The integration of other imaging and scattering modalities, such as monochromatic and μ-Laue x-ray beamlines at synchrotrons capable of producing detectable diffracted intensities in small volumes,

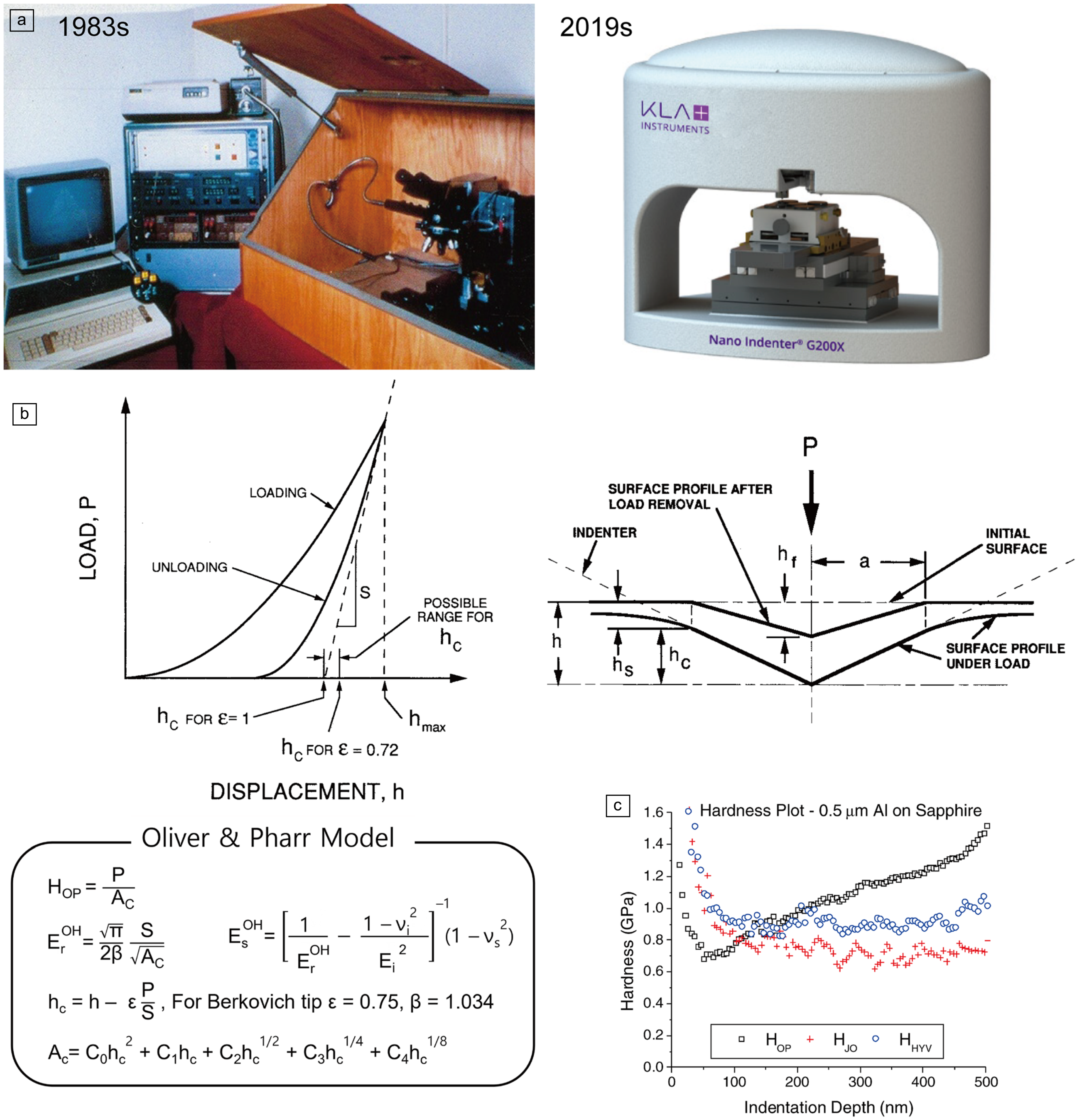

Figure 1. (a) The first commercial nanoindenter, Nano I - system[9] and recently developed nanoindenter, Nano Indenter® G200X of the KLA Corporation.[10] (b) Schematic illustration of the Oliver & Pharr (O&P) method.[5] E_s, E_i, ν_s, ν_i are Young's modulus and Poisson's ratio of the sample (s) and the indenter tip (i). (c) Hardness (H_{OP}, - H_{JO}, - H_{HYV}) versus indentation depth plot for 0.5-µm-thick Al thin films on sapphire substrates. Subscripts OP, JO, and HYV refer to the Oliver–Pharr model, the Joslin–Oliver model, and the Han–Yu–Vlassak model, respectively. Especially, - H_{JO} refers to the data for an elastically matched Al on glass substrate, which is plotted together to compare the counterparts with substrate mismatch.[6]

naturally occurred.[24–26] The attention focused on size effects in plasticity of single crystalline nanosized and other nanostructured materials (e.g., nanocrystalline or nanolaminated materials) previously described placed *in situ* testing squarely in the spotlight as a means of discovering new mechanisms and validating predictions from simulations. These include mechanical annealing of and source-mediated size effects of single crystalline metals, dislocation–grain-boundary interactions in oxides,[27] and the identification of thermally activated plasticity mechanisms by incorporating heating and cooling

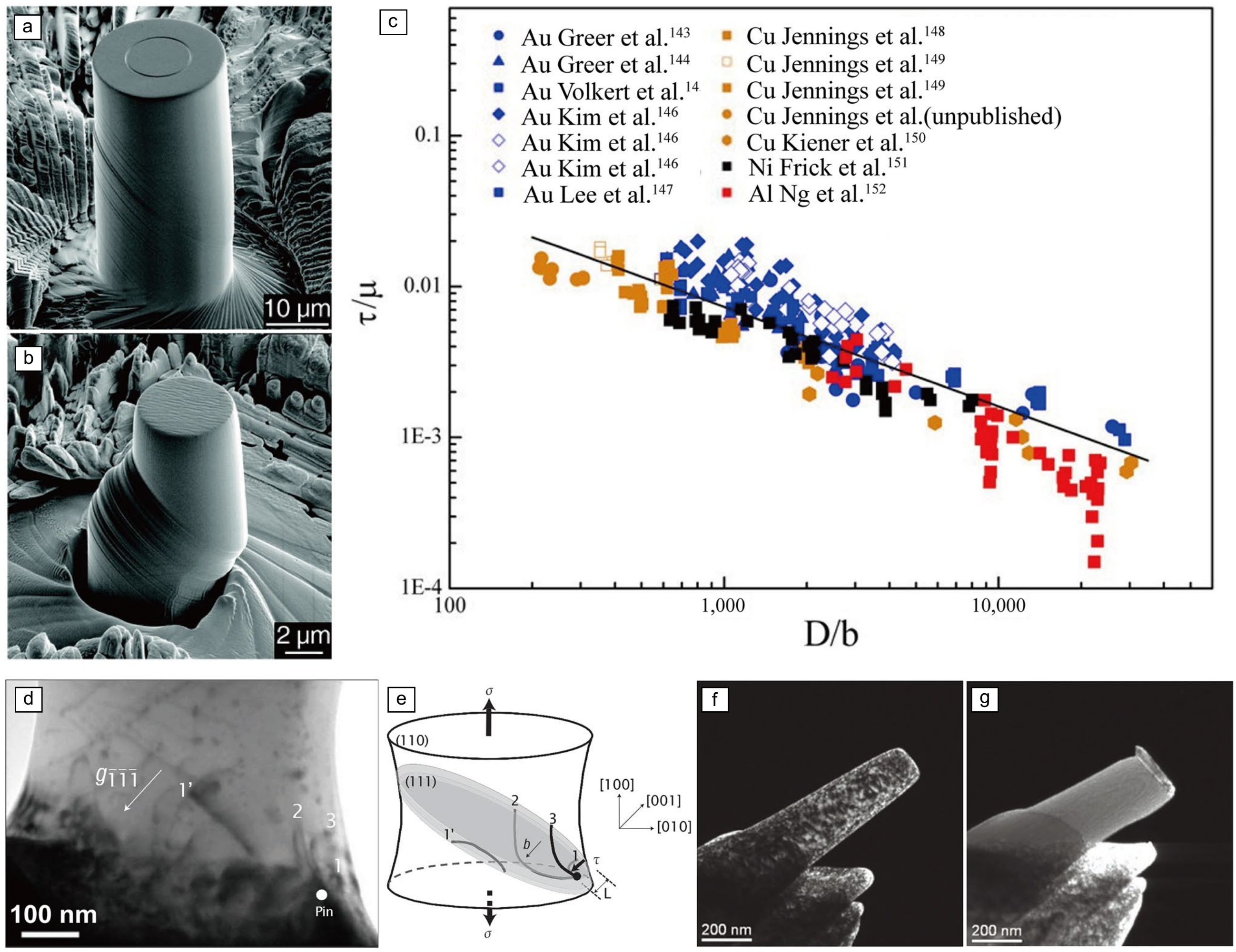

Figure 2. (a, b) Scanning electron microscope (SEM) images of Ni micropillars (a) tested to ~4% strain and (b) tested to ~19 percent.[3] (c) Normalized shear flow stress for most face-centered cubic metals micro-nanopillar test.[17] (d) Transmission electron microscopy (TEM) images showing the operation of single-armed sources and (e) schematic of the single-armed source and dislocation configuration of (d).[13] (f, g) Dark-field TEM images of *in situ* compression tests on 160-nm Ni pillars. (f) The pillar before the compression with the high initial dislocation density and (g) the same pillar after the compression which is a dislocation-starved state.[12]

capabilities concurrent with straining.[28,29] Microelectromechanical systems (MEMS)-based platforms[30] capable of tensile testing, either through thermal- or capacitive-based actuation or using clever mode-conversion (e.g., push-to-pull and "theta" devices[31]) emerged and enabled the extraction of a full property suite from a single experiment. Alongside important new scientific discoveries, these tensile experiments allowed for a critical examination of the influence that boundary conditions play at small scales.[32]

The most modern era of *in situ* testing is arguably at the nexus of enhanced characterization modalities, machine learning/artificial intelligence (ML/AI)-based analysis tools, and detectors producing large volumes of data. These advances capitalize on the convergence of ultrabright illumination sources (both electron and x-ray) and ultrafast and sensitive pixelated area detectors, greatly accelerating both the information that can be extracted during *in situ* testing and the amount of data generated. On one side of this spectrum lies exciting hardware advancements in scanning nanodiffraction and direct electron detectors within the TEM (known as 4D-STEM).[33] Because the full gamut of crystallographic, phase, lattice strain, and local electric and magnetic field information from the specimen is encoded in the diffraction information, a large number of details about the material can be deduced with the proper analysis *ex post-facto*. Bridging the other side of the spectrum are the vast computational and modeling toolkits developed to analyze information from both diffraction patterns and images, with the promise of high-throughput, multimodal data fusion, and data dimensional reduction motivating the increasing adoption of ML- and AI-based tools.[34,35] Examples of using *in situ* nanomechanical testing paired with 4D-STEM quickly emerged.[36] As an example of the power of combining ML tools and *in situ* testing, Song et al. recently overcame the challenges associated with image recognition

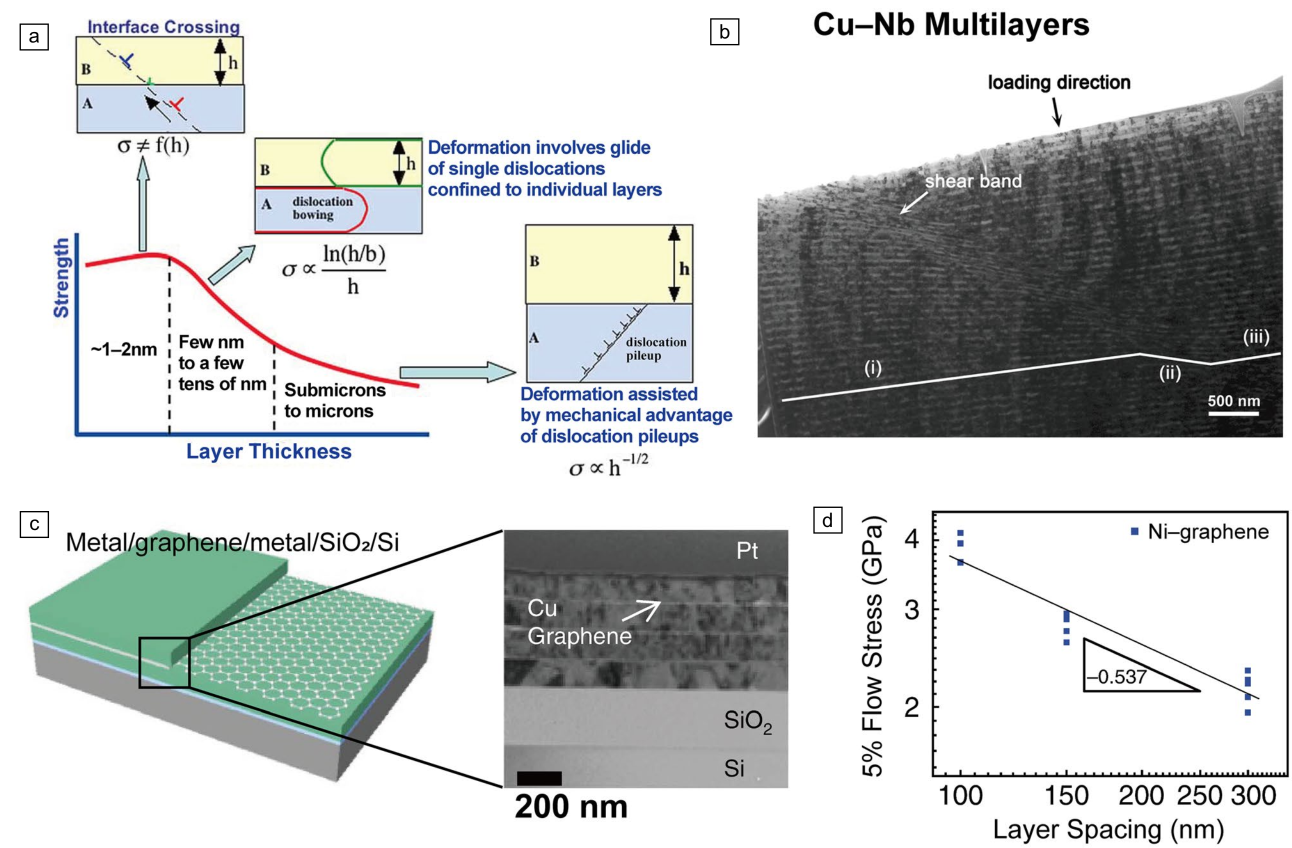

Figure 3. (a) The dislocation mechanisms of multilayer at different length scales.[18] (b) Transmission electron microscopy bright-field image of shear band formation in 40-nm Cu/40-nm Nb multilayer with {111}Cu//{110}Nb interface. The white line refers to the trace of the layers across the shear band, which shows the distortion within the shear band.[19,20] (c) Schematics of a metal–graphene multilayer and their micropillar compression testing. (d) The flow stresses at 5% plastic strain versus layer spacing plots of Ni–graphene multilayers.[22]

and detection of linear features using a deep learning model applied to *in situ* TEM sequences of gliding dislocations to quantify the depinning stresses of the obstacles landscape in the fcc Cantor high-entropy alloy and calculate full avalanche statistics[37] (**Figure** 4).

SEM-based *in situ* techniques have largely provided near-surface information about plastic slip via direct imaging, digital image correlation (DIC), and electron backscatter diffraction (EBSD). The latter two have made exciting and notable strides. First, DIC has advanced to allow for the direct measurement of plastic slip amplitudes and direction using correlation algorithms that quantify the discontinuities at surface slip traces across large areas of polycrystals and their important microstructural features, such as grain boundaries and triple/quadruple junctions. An exciting example is that of Stinville et al., where a large data set of slip localization across many important structural alloys was used to demonstrate how a single and reversed cycle of elasto-plastic loading was sufficient in predicting fatigue crack initiation at a large number of cycles.[39] Second, EBSD has made important advancements relevant to *in situ* testing beyond its initial application of orientation mapping: (1) lattice (elastic) strain mapping using high (angular)-resolution EBSD and advanced algorithms,[40] (2) single-defect identification using local orientational fields,[41] and more recently, (3) defect mapping using whole pattern- and band-specific sharpness quantification.[42] The integration of modern direct electron detectors in an SEM environment is a particularly promising avenue for future *in situ* studies.[43–46]

The lines between modalities in the TEM and SEM environments that will enhance *in situ* testing are beginning to blur in exciting ways. First, whereas diffraction information and imaging with specific diffraction conditions have long been considered the domain of S/TEM, advanced EBSD and electron channeling contrast imaging (ECCI)[47,48] are now readily implemented during *in situ* testing. Second and more recently, the use of transmission modalities on thin specimens in the SEM should be used to image defects such as dislocation and their dynamics, and the SEM platform offers practical advantages in terms of space for *in situ* instruments. Notable examples include the *in situ* determination of deformation mechanisms of Ni-based superalloys[49] and refractory multiprincipal element alloys[50] using STEM in the SEM (termed transmission SEM or TSEM), and the observation of stress-induced phase transformations using *in situ* transmission Kikuchi

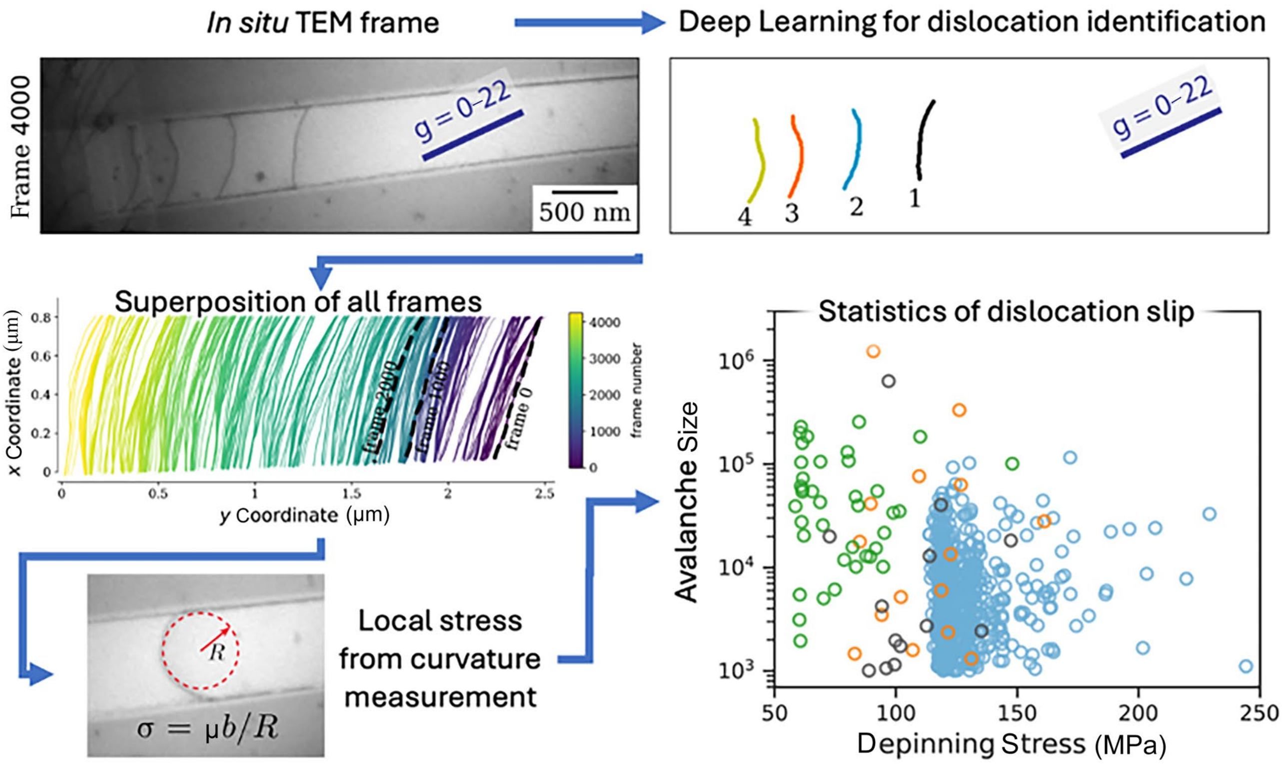

Figure 4. Combining *in situ* transmission electron microscopy (TEM) observations of dislocation glide with a deep learning model to track the morphology of dislocations as they traverse the slip plane. From measurements of local curvature, a large statistical database of obstacle depinning stress versus avalanche size was constructed.[38]

diffraction (TKD).[51] The continual improvement of electron columns, detectors, and multi-degree-of-freedom stages in the SEM will accelerate this blurring into hybrid electron microscopes (**Figure** 5), with tantalizing opportunities for micro- and nanomechanics.

Fracture testing: Bridging length scales

Methods for characterizing the fracture behavior of materials at the macroscopic length scale are well established. It is well understood that the influence of plastic deformation specifically, the ratio of the plastic zone size to the sample dimensions—introduces a length scale dependence in measured fracture toughness. Only when the sample size exceeds a certain threshold can intrinsic "materials properties" be reliably distinguished from length-scale-dependent "system properties." For brittle and semi-brittle materials, like most semiconductors and hard coatings, this critical sample size is well below the micrometer dimensions. Consequently, FIB-fabricated samples can be used to assess the fracture toughness of microsystems. The most common geometries with FIB-milled pre-notch are single cantilever bending,[53,54] clamped beam bending[55] and double cantilever beam bending (DCB),[56] and pillar splitting as a notch-free method to estimate the fracture toughness.[57] FIB-milled specimens are subsequently tested *in situ SEM* using a nanoindenter, theoretically enabling real-time observation of the fracture process. The fracture toughness is then determined based on the critical load at fracture, in combination with precise knowledge of the sample geometry and geometry-specific correction factors derived from finite element method (FEM) modeling.

One of the greatest challenges in the preparation of small-scale fracture specimens arises due to FIB-induced damage.[58] FIB-fabricated notch could exhibit changes in chemical composition (e.g., segregation), phase changes, amorphization, newly introduced crystal defects,[59] and residual stresses.[60] Reducing FIB-induced damage using noble gas ions, such as He, Ne, or Xe[4,61] is chemically advantageous; however, compared to Ga, it introduces new challenges, such as Ne bubble formation.[4] It is therefore advisable to consider the use of stable crack growth geometries to grow the crack into the unaffected region of the material and subsequently measure the local fracture toughness from this point. Mueller and co-workers[62] used a Chevron notch milled by the FIB and observed stable crack growth along the (111) plane in silicon, and they successfully initiated a propagating crack by applying cyclic loading using a micromanipulator, where the approach of formation of a fatigue precrack from a FIB-milled notch was used. DCB configuration is an alternatively stable geometry of Liu et al., although accurately

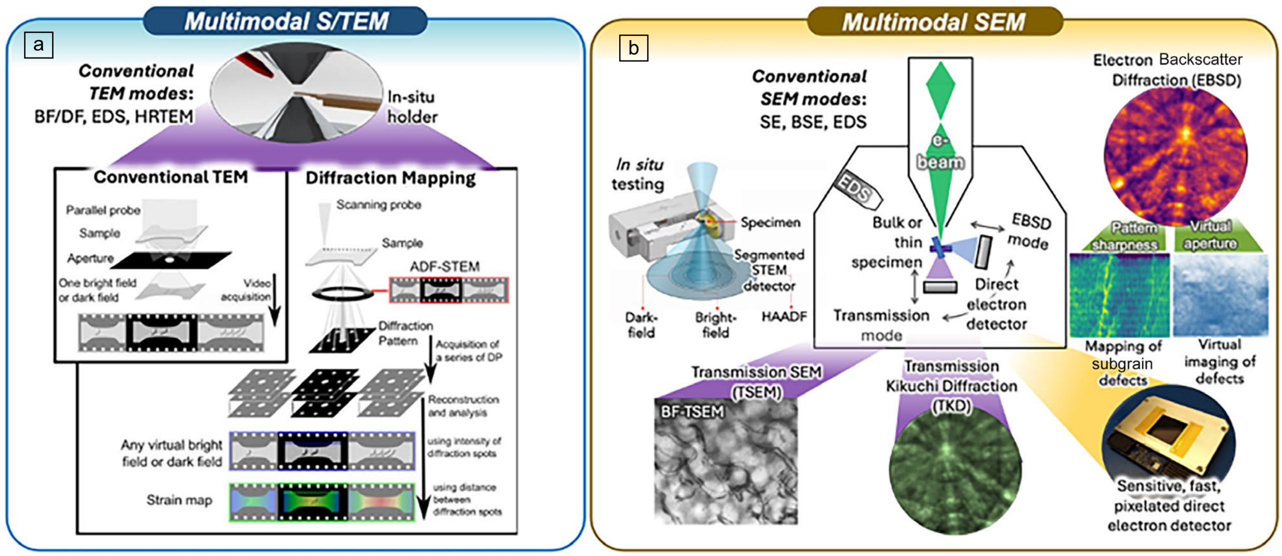

Figure 5. Multimodal electron microscopes. Expanding the capabilities of the electron microscope for *in situ* nanomechanics. (a) Modalities within scanning/transmission electron microscopy (S/TEM) platforms, both imaging and scanning electron nanodiffraction (4D-STEM) mapping, allowing for virtual imaging, strain mapping, and other analyses. Images taken and adapted from References 52 and 36. (b) Modalities within SEM platforms, including advanced EBSD approaches using direct electron detectors, transmission SEM (TSEM), and transmission Kikuchi diffraction (TKD). Abbreviations: bright field (BF), dark field (DF), energy-dispersive x-ray spectroscopy (EDS), high-resolution transmission electron microscopy (HRTEM), annular dark field (ADF), backscattered electron (BSE).

determining the interface fracture toughness using this approach requires a detailed understanding of the sample–indenter system, including factors such as contact friction. Sernicola[63] et al. used a wedge-shaped indenter to directly assess the energy release rate of grain-boundary fracture, and Okotete et al.[64] used a cantilever-based stable crack growth geometry to measure the toughness of the interface between a multicomponent carbide coating on a silicon wafer.

Geometries involving stable crack growth following crack nucleation at a FIB-fabricated notch enable the analysis of a fracture toughness value representative of FIB-free material, although such experiments are challenging. As early as a foundational study, Matoy et al.[54] proposed the use of the so-called bridge notches. In this approach, the crack is intended to nucleate at a material ligament and subsequently arrest. The resulting sharp precrack, located outside the FIB-affected zone, is then used to determine the fracture toughness upon catastrophic (final) fracture. The bridge notch concept, however, also presents a significant challenge: the stress intensity at the ligament prior to crack initiation differs from that at the sharp, arrested crack. Therefore, to determine the fracture toughness from a specimen containing a bridge notch, it is essential to verify whether crack arrest has occurred. This imposes stringent requirements on both the bridge geometry and the force resolution of the indenter. Only through optimized geometric design and the use of the latest generation of *in situ* indenters has this approach become feasible recently and reproducible.[65]

Linear elastic microfracture mechanics has been rapidly established and made application-ready over the past two decades. Challenges arising from FIB-based sample preparation can now be mitigated—or even completely overcome—through stable crack growth geometries. However, for widespread adoption, including industrial use in quality assurance, internationally accepted standards regarding sample geometry, applicable dimensions, and testing within the electron microscope are urgently needed.

Dynamic nanomechanical testing

With the establishment of nanomechanical characterization as a rapid tool for materials analysis, demand has grown for its application under extreme, application-relevant conditions. These include high and low temperatures, harsh chemical environments, and high-strain rate deformation.[66–68] In the context of high-rate deformation, nanomechanical techniques offer unique advantages: reduced cost and time of experiments, small sample sizes, and convenience through benchtop setups, unlike national-laboratory-scale testing facilities that are often required to reach extreme macroscale conditions. In response to this opportunity, several novel techniques have emerged, collectively spanning nearly 10 orders of magnitude in strain rate, into regimes where shock and hydrodynamic responses are relevant (see **Figure 6**).

The most robust and validated method enabling nanomechanical characterization in this domain is instrumented nanoindentation. Early systems were load-controlled devices[69] which reliably covered the quasistatic 10^{-3} to $\sim 10^{-1}$ s^{-1} strain rate regime. More recently, displacement-controlled devices and modified load-controlled systems

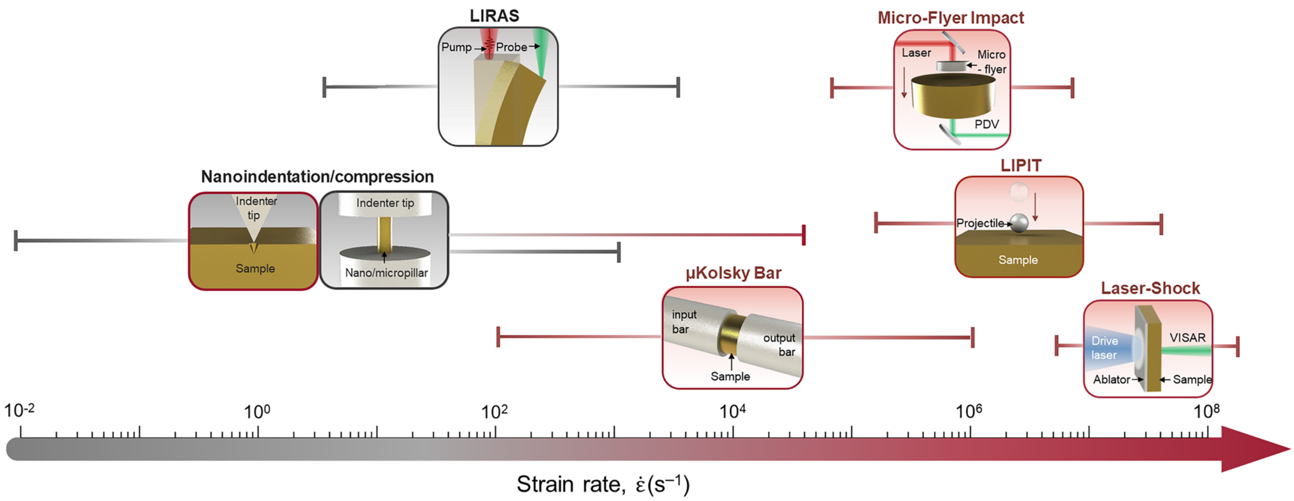

Figure 6. Overview of nanomechanical characterization techniques, organized by their approximate achievable strain rates. VISAR, velocity interferometer system for any reflector.

have expanded the range of testable strain rates. Displacement-controlled setups using piezoelectric actuators and load cells have reached 10^4 to 10^5 s^{-1},[70] while modified load-controlled systems with electromagnetic actuation and interferometric displacement sensing have achieved rates up to 10^4 s^{-1}.[69,71–73] While these rates are effective strain rates achieved within indentation procedures, some systems have enabled uniaxial compression at rates of 10^2 to 10^3 s^{-1}, a regime traditionally accessible via servo-hydraulic tools or split Hopkinson pressure bars (SHPBs) at the macroscale.

An emerging alternative technique consists of a miniaturization of the well-established macroscopic split Hopkinson pressure bar method.[74] In this setup, a striker impacts an input pressure bar, transmitting a stress wave through a sample and into an output bar. Strain gauges on the bars capture wave profiles that are analyzed to reconstruct the sample's stress–strain response.[75] While standard SHPB setups are typically limited to strain rates $\leq 10^3$ s^{-1} due to equilibrium and wave dispersion issues, miniaturized versions have reached rates up to $\sim 10^6$ s^{-1}.[76,77] This is due to two key advantages: (1) microscopic samples reach equilibrium more rapidly and (2) small-diameter bars propagate high-frequency/rate signals more effectively. However, miniaturization introduces challenges—optical measurement techniques must replace strain gauges in submillimeter bars, and sample fabrication becomes significantly more complex.

Alternatively, other high-rate techniques sacrifice full stress–strain reconstruction to reach even higher strain rates through impact-based methods. One such technique is the laser-induced particle impact test (LIPIT), where an ultrafast pulsed laser ablates a metallic coating to launch microparticles toward a sample.[78,79] Ultrafast imaging captures impacts at velocities up to ~1 km/s, enabling measurement of energy absorption,[80] restitution coefficients, and through postmortem analysis, properties such as hardness.[81] Over more than a decade, LIPIT has enabled characterization of a variety of materials, including metals,[81–83] ceramics,[84] and 2D materials under strain rates of 10^6 to 10^8 s^{-1}.[85] A related technique is the laser-driven flyer plate method, in which thin metallic disks (25–100 µm) are launched at speeds of 1–4 km/s for shock compression experiments.[86] Ultrafast imaging and techniques such as photon Doppler velocimetry (PDV) enable time-resolved measurements of sample responses, such as spall strength in metals and alloys.[87,88]

While the aforementioned methods involve direct contact through probes or projectiles, new noncontact approaches have emerged to characterize materials at even higher rates. One such approach uses laser-induced shock loading, where a high-energy, picosecond-range laser pulse generates planar or concentric shocks in a target material.[89] Characterization is performed through diagnostic laser pulses or post-shock analysis, including assessments of chemical changes,[90] providing insights into highly dynamic, nonlinear behavior under extreme conditions. Another recent noncontact approach, laser-induced resonant acoustic spectroscopy (LIRAS), uses multidirectional laser pumps and probes to determine full elastic properties of materials by measuring resonant frequencies in micropillars[91] While this technique operates at lower energies than shock-based methods, it enables precise characterization of dynamic elastic behavior without contact.

Altogether, these advances now enable nanomechanical characterization across a strain rate spectrum spanning at least 10 orders of magnitude. While quasi-static methods are well-established, dynamic techniques present new frontiers for materials research. Each high-rate method offers unique capabilities and limitations, and future work in dynamic nanomechanics will benefit from the development of standardized data analysis and interpretation frameworks, which remain lacking for these complex regimes.

Characterization of nano- and micro-architected materials

Architected materials, also known as mechanical metamaterials, consist of engineered 3D nano- and microstructures designed to exhibit tailorable effective materials properties. Emerging in the early 2010s, they offered a more tunable alternative to nanoporous foams produced via dealloying[92] or inverse opals formed through the self-assembly of spherical components.[93] Their development was largely driven by high-resolution additive manufacturing techniques such as two-photon lithography (TPL).[94] Sacrificial 3D polymeric templates were used to deposit conformal nanoscale coatings of ceramics or metals, and the hierarchical structuring that makes use of size-dependent strength and plasticity of nanoscale metals[95] and ceramics[96,97] enabled for otherwise unachievable mechanical properties. For example, the transition in brittle to ductile transition of nanoscale ceramics allowed for enhanced ductility and recoverability in ceramic hollow-beam lattices.[98] Due to their high porosity and low stiffness, these materials were ideally suited for instrumented nanoindentation tools, especially with their ability to provide *in situ* SEM direct observation of nonlinear responses and failure mechanisms, correlating stress–strain responses to global deformation modes[98] (see **Figure** 7).

Curved-shell architectures, such as mathematically defined triply periodic minimal surfaces (TPMSs)[102] without sharp stress concentrations, symmetry-breaking and defect-tolerant structures, such as those based on spinodal decomposition with tunable morphologies[105,106] as well as beam-based lattices with functional gradients or embedded heterogeneities have been reported. More recently, computer-optimized nanoarchitectures have been proposed to further enhance material performance.[110] The dynamic behavior of architected materials, especially under high-strain rate conditions, remains a growing field of study. Investigations now span acoustic responses[109,111] particle-impact mitigation,[109,112] dynamic compaction, and shock mitigation.[113] With advances in nanoscale fabrication, including the use of previously inaccessible materials such as piezoelectric ceramics[114] glasses,[115] metals[116] and composites,[117] current and future explorations will be focusing on coupled responses or nonlinear deformation mechanisms driven by architectural complexity and small length scales. In this context, advances in nanomechanical characterization—particularly *in situ* techniques—will play an essential role in unlocking new discoveries in this field within the next decade.

Multiscale modeling, ML, and AI in nanomechanics

With the growing accessibility of AI and quantum computing, the exploitation of rich experimental data sets from a variety of nanomechanical testing methods opens the possibility to significantly reduce the time required for materials discovery and/or for understanding structure/property correlations in advanced materials. High-speed nanomechanical mapping, for example, becomes a primary input for supervised and unsupervised learning algorithms that interpolate and classify mechanical behavior across heterogeneous phases or gradients,[118,119] especially in crucial scenarios where understanding their performances needs a tight coupling and correlating efforts across diverse other characterization techniques (e.g.,

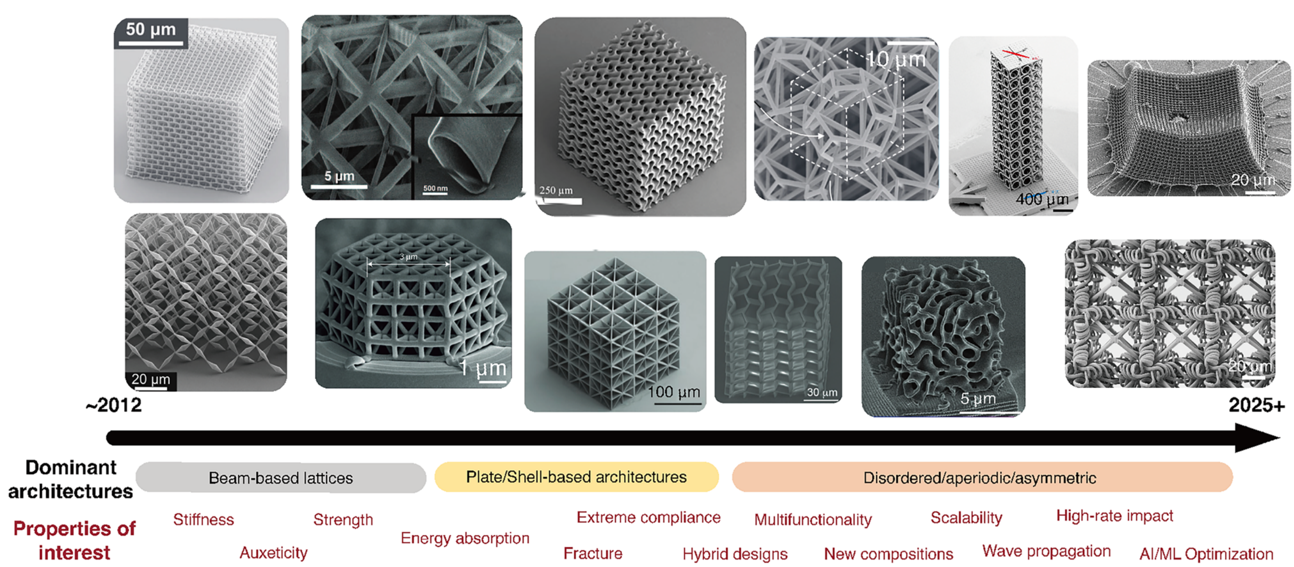

Figure 7. Evolution of nano- and micro-architected materials research over the last ~15 years. Initial research questions revolved around periodic beam-based lattice architectures,[94,99,100] followed by plate- and shell-based morphologies,[101–103] and more recently focusing on the role of aperiodicity and disorder in these materials.[104–106] Additionally, while initial efforts addressed questions about the linear properties of these materials, recent directions are pursuing an understanding of nonlinear properties,[107] failure, and responses under extreme conditions.[108,109]

EBSD, energy dispersive x-ray spectroscopy(EDX), pillar splitting[120]). Deep learning models have also been trained on high-speed indentation data sets to identify features such as pop-in events and to convert force–displacement data to full stress–strain behavior.[121,122] Similarly, Bruno et al. combined EBSD with indentation maps using Gaussian mixture and k-means clustering to associate mechanical phases with crystallographic information in TRIP steels.[123] Vignesh et al. demonstrated the effectiveness of millisecond-scale indentation combined with unsupervised clustering to resolve the mechanical response of thermally grown oxide, ceramic topcoat, and bond-coat regions in thermal barrier coatings.[124] Additionally, correlative multi-technique approaches have shown the ability to directly link local mechanical behavior to microstructure. Magazzeni et al. combined nanoindentation with EBSD and electron micro-probe analysis (EPMA) in titanium alloys, revealing strong correlations between hardness, crystallographic orientation, and local chemistry.[125] Together, these studies demonstrate that the integration of nanoindentation with AI and correlative microscopy is maturing into a robust methodology for unraveling microstructure–property relationships in complex systems.

In the fields of multiscale materials modeling, ML methods are increasingly being used as powerful and effective "amplifier" to enrich fundamental modeling databases at reduced computational cost. As an example, ML can be used to augment existing density functional theory (DFT) databases to develop new formulations of high-entropy materials (HEMs)[126] or to develop universal machine-learned interatomic potentials (MLIPs) that could be used to increase the time and scale domain of molecular dynamics (MD) simulations.[127,128] When trying to understand plasticity and fracture at the nanoscale, the proper simulation of the role of defects and imperfections (e.g., dislocations and microcracks) becomes critical for a proper understanding of failure mechanisms. Here, the use of MLIPs can be crucial for the increase of accuracy at reduced computational time.[129] At mesoscopic scales, ML-based tools are being increasingly applied to improve our understanding of the mechanical behavior of polycrystalline materials (and more in general granular media), given their ability to extract microscale mechanical characteristics directly from raw data with reduced preliminary assumptions.[130]

Even when dealing with continuum models, surrogate models based on machine learning have been shown to effectively solve the inverse indentation problem, enabling direct estimation of elastoplastic parameters from single P–h curves.[131] Some recent studies have demonstrated a further integration of experimental nanomechanical testing with computational modeling and advanced data-driven analysis, closing the triangle between experiment, theory, and AI. Lyu et al. combined AFM-based nanoindentation experiments with finite element (FE) simulations and machine learning to determine the mechanical response of ultrathin freestanding ferroelectric lead zirconate titanate (PZT) films.[132] When applied to experimental nanoindentation data, the model enabled the simultaneous extraction of multiple unknowns (modulus, pretension, thickness) with reduced computation times. This work demonstrates how AI-enhanced nanoindentation can resolve mechanical behavior in freestanding nanoscale membranes where standard continuum assumptions break down.[132]

At the atomistic level, Ge et al. developed an integrated framework combining large-scale MD simulations with MLIPs and AI-based phase classification to study nanoindentation-induced phase transitions in silicon.[119] This combined MD–ML approach provided unprecedented insight into the mechanisms of pressure-induced phase changes during indentation, directly bridging atomistic modeling with experimental observations of phase transitions in silicon.[133]

Athanasiou et al. presented a fully integrated experimental–computational–ML methodology applied to indentation pillar-splitting experiments for fracture toughness evaluation in brittle ceramics.[134] The authors coupled *in situ* microscale indentation fracture tests with cohesive zone finite element modeling to simulate crack propagation, which was further augmented by Gaussian process regression to model the critical transition from stable to unstable cracking. The resulting integrated framework accurately predicted the critical fracture load and allowed quantitative extraction of toughness values despite complex instability phenomena that limit conventional pillar-splitting analysis.

In the broader context of inverse nanoindentation, Jiao et al. developed a machine learning-based surrogate modeling framework to address the long-standing challenges of extracting elastoplastic properties from load–displacement curves.[131] By training neural networks on FE-simulated data sets that included pileup and sink-in effects, they directly predicted yield strength, hardening exponent, and other plastic parameters, while simultaneously addressing the inherent nonuniqueness of traditional indentation inversion. This highlights the growing capacity of AI-based models to resolve complex inverse problems in nanomechanical characterization that would otherwise remain ill-posed.[131]

Despite these advances, a relevant bottleneck can still be represented by the lack of interoperability between data from experimental platforms or modeling environments. In fact, the definition of a shared ontological framework is becoming a central issue toward the establishment of adaptive and harmonized modeling/characterization/AI protocols (see **Figure** 8). Without common vocabularies and semantic structures, the flow of information between characterization, simulation, and AI remains fragmented and nonscalable. To address this, efforts are underway to develop digital ecosystems where data from different sources can be integrated within open, application programming interface (API)-based environments. The evolution toward semantic web technologies (Web 3.0) represents a promising direction in this context,[135] allowing materials knowledge to be encoded in machine-readable formats and made available for automated reasoning and discovery. Ultimately, the digitalization

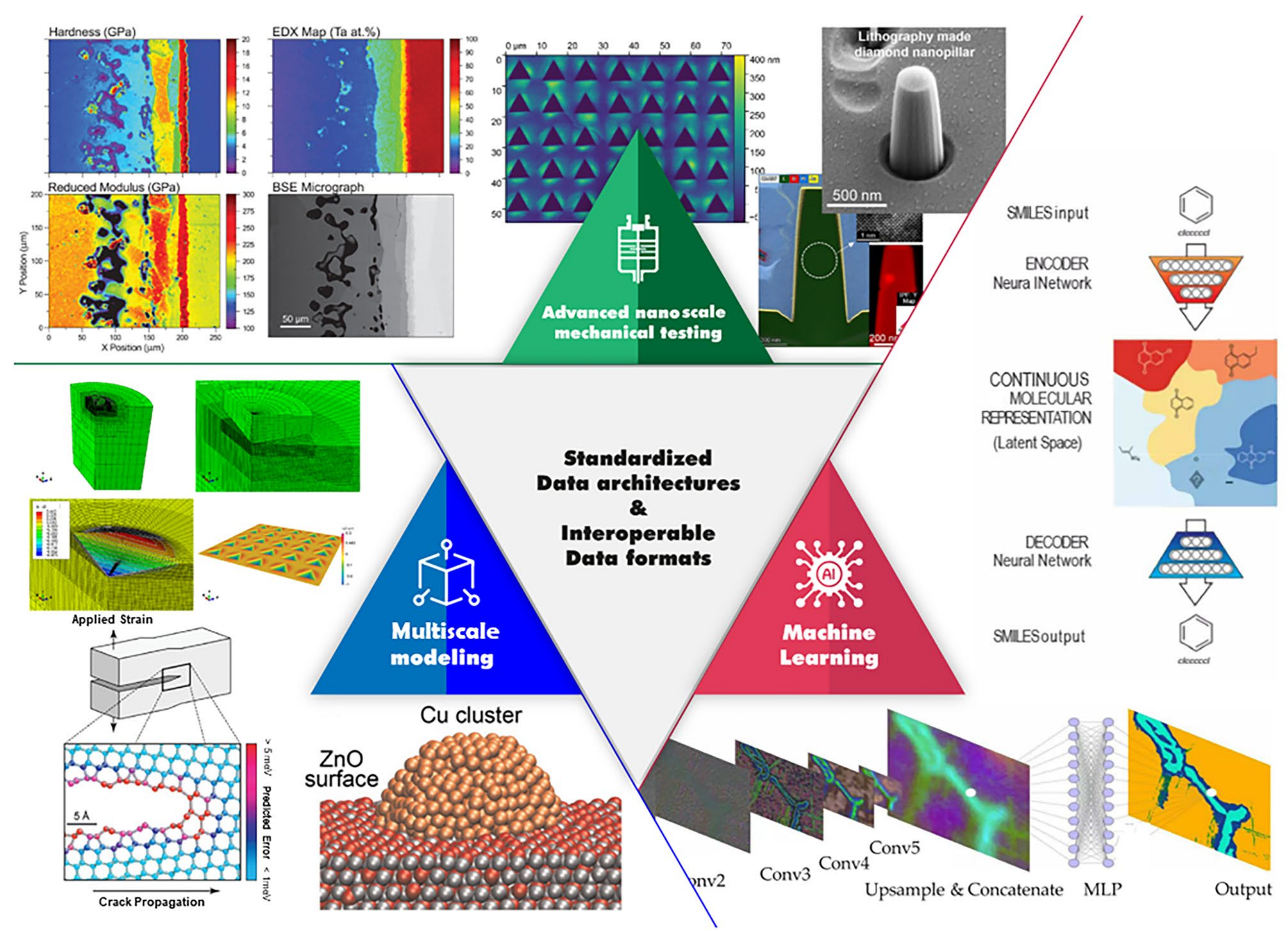

Figure 8. A vision for integrated and adaptive modeling/characterization/machine learning tools, where standardized and interoperable data allow for rapid interexchange of information across the three domains. Reproduced from DeCost et al.[136] (© 2019 Oxford University Press), Gómez-Bombarelli et al.[137] (© 2018 American Chemical Society, published under the ACS AuthorChoice license), and Wheeler et al.[138] (© 2022 Wiley, published under the Creative Commons CC BY-NC-ND 4.0 license); adapted from Rossi et al.,[139] Jain et al.,[140] Bartók et al.,[141] and Dattila et al.,[142] with permission from the respective publishers.

of materials development hinges on the ability to combine experimental data, simulations, and AI into coherent and adaptive workflows. Such integration will enable the realization of FAIR (findable, accessible, interoperable, and reusable) data architectures that support the design of nano-enabled materials for high-impact applications. Importantly, these frameworks offer a route to reduce the need for exhaustive physical testing, facilitating faster, more cost-effective, and more sustainable materials innovation.

Future directions and challenges

The nanomechanics field has evolved into a multidisciplinary platform that enables probing, understanding, and designing material behaviors at unprecedented spatial and force resolutions. As we move forward, emerging opportunities lie in integrating nanomechanical methods with ML and *in situ* characterization tools for new materials discovery and analysis of deformation mechanisms across different length scales. Future research will likely focus on quantifying mechanics in complex, dynamic, and often extreme environments, such as in high-temperature aerospace structures under cyclic mechanical and aerodynamic loads. Challenges still remain in establishing robust multiscale frameworks that bridge spatial and temporal disparities as well as in achieving high reproducibility across diverse experimental platforms, and in effectively correlating nanoscale deformation behavior with macroscopic materials properties. Nevertheless, with continued innovation in instrumentation, modeling, and interdisciplinary collaboration, the nanomechanics field is well-positioned to not only deepen the mechanistic understanding of new materials, but also drive breakthroughs in a variety of engineering applications such as quantum materials, flexible electronics, soft robotics, and beyond.

Conclusion

Deformation mechanisms in small-scale materials differ from the bulk counterparts due to the confinement of dislocations within the small volume, and the nanomechanics community has diligently pushed forward in the development of novel characterization tools that have allowed for the uncovering of new phenomena that govern the mechanical properties of small-scale materials. Studies of thin films were extended to a more challenging study of nanoscale individual structures, and the accrued knowledge of the mechanical properties of nanoscale materials allowed for the development of materials systems with extreme strengthening effects, such as 2D nanolayered composites as well as 3D-nanoarchitected structures. Recent advances in AI and machine learning-based characterization and modeling now allow for effective screening for nanomechanical properties and analysis of the underlying deformation mechanisms. The wealth of knowledge and database will open up an unexplored realm to develop new mechanical metamaterials for futuristic applications, such as in outerspace materials for extreme environments. The nanomechanics community has and will continue to be at the frontier of discovering novel small-scale materials that suit the needs and interests of the evolving technological interests.

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Author contributions

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Conflict of interest

On behalf of all authors, the corresponding author states that there is no conflict of interest.

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