

Article

Fluence-Dependent Multimodal Response of NdGaO₃(110) Single Crystals to 147 MeV Kr Ions

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Abstract

This exploratory study compares one pristine NdGaO₃(110) crystal with one crystal irradiated at 1×10^{11} ions cm⁻² and one crystal irradiated at 1×10^{12} ions cm⁻² using 147 MeV ⁸⁴Kr ions. Because each condition is represented by a single independent specimen, specimen-to-specimen variability is confounded with the irradiation condition, and no specimen-level statistical inference is made. Symmetric X-ray diffraction, condition-averaged confocal micro-Raman spectroscopy, and UV–Vis–NIR transmission were used to compare surface-normal lattice response, local vibrational line shapes, and radiation-induced optical attenuation. The nearly angle-independent XRD shift at 1×10^{11} ions cm⁻² is dominated by a common angular offset, whereas the two surviving harmonics at 1×10^{12} ions cm⁻² give a model-conditioned estimate $\varepsilon_{110} = +0.509 \pm 0.040\%$. At the higher fluence, the integrated intensities captured in the coupled θ – 2θ condition decrease to $9.35 \pm 0.46\%$ for (110) and $1.29 \pm 0.06\%$ for (220), while the (220) FWHM ratio reaches 7.83 ± 0.73 . These fit-derived errors do not include specimen alignment or between-specimen variability. The archived condition-averaged Raman spectra retain Pbnm-like vibrational groups, while the fitted FWHM values of the 168, 214/215, and 449–470 cm⁻¹ features increase by 15.7%, 19.4%, and 14.8%. The bulk-integrated Nd³⁺ 4f–4f maxima remain stable within the wavelength sampling, whereas the effective R_p-normalized differential attenuation at 275–285 nm reaches 388.7 cm⁻¹. The data support an exploratory description of a strained and diffraction-heterogeneous crystalline layer; complete amorphization, quantitative mosaicity, a damage threshold, track dimensions, and a microscopic defect identity are not established.

Keywords: NdGaO₃; swift heavy ions; krypton irradiation; X-ray diffraction; Raman spectroscopy; differential attenuation; lattice strain; GaO₆ octahedra



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1. Introduction

NdGaO₃ is a distorted rare-earth perovskite with orthorhombic Pbnm symmetry and a three-dimensional network of corner-sharing GaO₆ octahedra [1–3]. Cooperative octahedral tilting results in pronounced crystallographic, magnetic, and thermoelastic anisotropies, including direction-dependent lattice parameters and thermal expansion [4–9]. These properties make NdGaO₃ an important single-crystalline substrate for orientation- and strain-controlled epitaxial growth [10]. Beyond its conventional role as a substrate, NdGaO₃ has attracted interest for terahertz and spintronic applications, exhibiting magnetic-field-induced Zeeman excitations, THz phase modulation, birefringence, and dichroism [11–13], while spin Hall magnetoresistance at the Pt/NdGaO₃ interface demonstrates its potential for paramagnetic spintronic heterostructures [14].

The (110) surface is widely used as a structural template for functional oxides. Surface preparation, termination, and oxygen coordination influence nucleation, interfacial stoichiometry, and strain transfer, while NdGaO₃ supports epitaxial superconducting and conducting heterostructures [15–18]. Radiation-induced changes in the substrate may therefore modify the boundary conditions imposed on an overlayer even when the average substrate phase remains identifiable.

NdGaO₃ also has a strongly anisotropic optical and electronic response. Generalized ellipsometry and electronic-structure calculations resolve direction-dependent dielectric functions and high-energy band-to-band transitions [19,20]. Because Nd³⁺ is a stoichiometric constituent, the transmission spectrum contains intense crystal-field-split 4f–4f manifolds and high-lying rare-earth transitions [21,22].

Raman spectroscopy provides a local probe of the same distorted framework. Polarized measurements, lattice-dynamical calculations, and later tensor-resolved work establish the Pbnm-active mode set and relate low-frequency bands to collective distortions, intermediate modes to oxygen-cage rotations, and upper modes to Ga–O stretching [23–26]. Apparent line positions and intensities depend on polarization and crystallographic azimuth, which requires caution when unresolved envelopes are analyzed without full tensor control.

In the swift-heavy-ion regime, electronic stopping can exceed nuclear stopping by several orders of magnitude. The rapid transfer of electronic excitation to the lattice can generate transient thermal spikes, point defects, residual stress, and track-associated disorder; the final state depends on topology, elastic constraint, redox flexibility, and recovery kinetics [27–29]. A single probe cannot separate all contributions: coupled θ – 2θ diffraction is sensitive to long-range registry, Raman spectroscopy to local vibrational disorder, and optical transmission to electronic defect states.

This work presents a descriptive comparison of one pristine NdGaO₃(110) specimen and one specimen at each of two irradiation fluences, 1×10^{11} and 1×10^{12} ions cm^{−2}. The aim is to compare the surface-normal lattice response, Raman line-shape evolution, and radiation-induced optical attenuation without extracting powder-domain sizes or an unsupported amorphous fraction. Because only two irradiated fluences and no independent specimen replicates were available, no damage threshold, saturation law, or ion-track interaction threshold is inferred.

2. Materials and Methods

2.1. Samples, Irradiation, and SRIM Calculations

Commercial NdGaO₃ single-crystal substrates were supplied by MaTeck GmbH (Juelich, Germany) and grown by the Czochralski method. The nominal dimensions were $10 \times 10 \times 0.5$ mm³. The polished surface was oriented parallel to (110) within $\pm 0.5^\circ$, and the manufacturer-reported density was 7.57 g cm^{−3}. One independent specimen was used for each condition: pristine, 1×10^{11} ions cm^{−2}, and 1×10^{12} ions cm^{−2}. The specimens

were not measured before and after irradiation as paired samples, and no independent specimen replicates were available. Consequently, specimen-to-specimen variability is inseparable from irradiation condition, and the series is treated as an exploratory descriptive comparison rather than a statistically replicated fluence-response experiment. Irradiation was performed at the DC-60 heavy-ion accelerator of the Institute of Nuclear Physics, Astana, Kazakhstan. The two irradiated specimens were exposed to 147 MeV $^{84}\text{Kr}^{15+}$ ions at normal incidence to the (110) surface under nominal room-temperature conditions; the specimen temperature was not monitored in situ.

The provenance of the irradiation metadata is distinguished in Table 1. During revision, the authors supplied additional operating information for this irradiation series: a 15+ charge state, an approximate total electrical beam current of 25 nA over a scanned area of approximately 14 cm², electromagnetic beam scanning in irradiation channel No. 3, and a chamber pressure of approximately 6×10^{-6} Torr. These details supplement the initially incomplete specimen metadata. They are reported operating conditions clarified during revision, not values extracted from a recovered time-resolved beam log.

Table 1. Specimen and irradiation parameters, with the source and status of each quantity.

Parameter	Value	Source/Qualification
Material	NdGaO ₃ single crystal	Czochralski-grown, MaTeck
Surface	(110) $\pm 0.5^\circ$	Polished; manufacturer specification
Dimensions	$10 \times 10 \times 0.5 \text{ mm}^3$	Nominal specimen dimensions
Ion and energy	$^{84}\text{Kr}^{15+}$, 147 MeV	Normal incidence; charge state clarified by the authors during revision
Nominal fluences	1×10^{11} and $1 \times 10^{12} \text{ ions cm}^{-2}$	One specimen per fluence; separate pristine reference
S_e/S_n	19.84/0.0515 keV nm ⁻¹	SRIM stopping values; $S_e/S_n \approx 385$
R_p	10.95 μm	SRIM projected range
Facility	DC-60, irradiation channel No. 3	Institute of Nuclear Physics, Astana, Kazakhstan
Total beam current	$\approx 25 \text{ nA}$	Reported total electrical current; author clarification during revision
Scanned area	$\approx 14 \text{ cm}^2$	Reported irradiation area; not the scanner's maximum target area
Mean current density	$\approx 1.79 \text{ nA cm}^{-2}$	Calculated from total current / scanned area
Mean ion flux	$\approx 7.43 \times 10^8 \text{ ions cm}^{-2} \text{ s}^{-1}$	Calculated from current, scanned area, and the 15+ charge state
Nominal exposure times	$\approx 135 \text{ s}$; $\approx 1346 \text{ s}$	Calculated for 1×10^{11} and $1 \times 10^{12} \text{ ions cm}^{-2}$, respectively; not logged durations
Scanning method	Two-dimensional electromagnetic scanning	Orthogonal magnetic deflection of the beam over stationary specimens
Typical scanning frequencies	≈ 110 and 230 Hz	Typical operating pair; specified range 85–300 Hz; not a run-specific record
Spatial uniformity specification	Non-uniformity $\leq 5\%$	Scanner specification for targets up to $50 \times 50 \text{ mm}^2$; not an absolute fluence uncertainty or a measurement for this run
Chamber pressure	Vacuum, $\approx 6 \times 10^{-6} \text{ Torr}$	Reported approximate pressure; author clarification during revision
Absolute fluence uncertainty	Run-specific estimate unavailable	Distinct from the scanner's $\leq 5\%$ spatial non-uniformity specification
Specimen temperature	Nominal room-temperature conditions	No in situ temperature monitoring; beam-induced heating was not quantified

Using the reported total current, scanned area, and charge of 15 elementary charges per ion gives a calculated area-averaged current density of approximately 1.79 nA cm^{-2} and an average ion flux of approximately $7.43 \times 10^8 \text{ ions cm}^{-2} \text{ s}^{-1}$. The corresponding nominal exposure times for 1×10^{11} and $1 \times 10^{12} \text{ ions cm}^{-2}$ are approximately 135 and 1346 s, respectively. These times were calculated from the nominal fluences and mean flux, assuming constant area-averaged exposure; they are not independently logged irradiation durations.

The channel No. 3 scanner uses magnetic deflection in two orthogonal directions. Its typical operating frequencies are approximately 110 and 230 Hz, within a specified range of 85–300 Hz; the different frequencies produce a two-dimensional irradiation pattern. The system is specified for stationary targets up to $50 \times 50 \text{ mm}^2$ with particle-distribution non-uniformity no worse than 5%. These are standard operating characteristics and a scanner specification, not a run-specific frequency log or uniformity measurement. The 14 cm^2 area used in the flux calculation is the reported scanned area, not the maximum target area. A run-specific absolute fluence uncertainty and an independent uniformity map were not available. The $\leq 5\%$ specification is not treated as an absolute fluence uncertainty, and no quantitative assessment of beam-induced heating is claimed because specimen thermometry was not performed.

SRIM-2013 simulations used an atomic ratio Nd:Ga:O = 20:20:60 and the manufacturer-reported density [30]. The electronic and nuclear stopping powers were 19.84 and $0.0515 \text{ keV nm}^{-1}$, giving $S_e/S_n \approx 385$. The projected range was $R_p = 10.95 \text{ }\mu\text{m}$, with longitudinal and lateral straggling values of 0.591 and $0.744 \text{ }\mu\text{m}$. The SRIM values are used as depth and stopping descriptors rather than as direct measurements of track radius or displacement density; the general limitations of SRIM-based damage estimates were considered [31].

2.2. X-Ray Diffraction and Harmonic Analysis

Structural measurements were performed with a Bruker D6 PHASER diffractometer (Bruker AXS GmbH, Karlsruhe, Germany) equipped with a Cu-anode source operated at 40 kV and 15 mA. Coupled symmetric θ – 2θ scans were collected from the flat (110) surface over $2\theta = 10$ – 92° using a step of 0.0547° . Interplanar spacings were calculated with the Cu $K\alpha_1$ wavelength $\lambda = 1.540593 \text{ }\text{\AA}$, while the Cu $K\alpha_1/K\alpha_2$ doublet was represented explicitly during local profile fitting. Each reflection was described with a doublet-compatible pseudo-Voigt profile and a local background; no global background subtraction was applied to the full pattern [32].

The specular sequence from a (110)-oriented orthorhombic crystal is (110), (220), and (330). These harmonics probe one reciprocal-lattice direction and do not provide three independent unit-cell parameters. The effective d_{110} spacing and a common angular offset Δ_0 were therefore obtained from a joint harmonic model:

$$2\theta_{n,obs} = 2\arcsin\left(\frac{n\lambda}{2d_{110}}\right) + \Delta_0, \quad n = 1, 2, 3 \quad (1)$$

The surface-normal strain was evaluated relative to the pristine joint-fit spacing:

$$\varepsilon_{110} = \frac{d_{110,irr} - d_{110,0}}{d_{110,0}} \quad (2)$$

Integrated areas and FWHM values were normalized to the corresponding pristine reflections. The reported uncertainty bars are propagated 1σ local-profile fitting errors; they are not specimen-to-specimen standard deviations. Peak broadening in the symmetric θ – 2θ scan is compatible with a combined contribution from a depth-dependent d-spacing distribution, specimen curvature, static disorder, and/or mosaic tilt, but these

contributions cannot be separated without rocking curves, reciprocal-space maps, and asymmetric reflections. Williamson–Hall and Scherrer analyses were not applied to the oriented single-crystal data.

Local XRD fit quality and residuals are reported in Supplementary Figure S1 and Table S1. The diagnostic pseudo-Voigt doublet fits give $R^2 = 0.9944 - 0.9997$ and normalized RMSE = $0.49 - 2.25\%$. The pristine and 1×10^{11} ions cm^{-2} harmonic fits have one residual degree of freedom; the two-reflection, two-parameter 1×10^{12} ions cm^{-2} fit has none, so a residual goodness-of-fit statistic is not defined for that condition. No external angular calibration standard or repeat specimen-realignment scans were acquired in the same series. A nominal 3σ fit-based strain sensitivity of approximately 0.033% follows from the propagated low-fluence uncertainty, but this is not a metrological detection limit.

2.3. X-Ray Information Depth

The XRD information depth was compared with the SRIM range using the linear attenuation coefficient $\mu \approx 1.85 \times 10^3 \text{ cm}^{-1}$, calculated from the elemental mass-attenuation coefficients tabulated by NIST at the Cu $K\alpha$ photon energy [33]. In symmetric geometry, the depth weighting is

$$I(z) \propto \exp\left(-\frac{2\mu z}{\sin \theta}\right) \quad (3)$$

The depth containing a fraction p of the diffracted signal is

$$z_p = -\frac{\sin \theta \ln(1 - p)}{2\mu} \quad (4)$$

For $p = 0.95$, the calculated values are 1.62 , 3.23 , and $4.85 \text{ }\mu\text{m}$ for (110) , (220) , and (330) , respectively. All are smaller than $R_p = 10.95 \text{ }\mu\text{m}$. Thus, within the ideal attenuation model, the symmetric XRD signal is dominated by the ion-modified depth interval. These XRD information depths are method- and angle-specific and must not be transferred to Raman or optical transmission, which have different sampling volumes.

2.4. Raman Acquisition and Line-Shape Analysis

Micro-Raman spectra were acquired at room temperature from the (110) surface using a TriVista CRS system (Princeton Instruments, Acton, MA, USA) operated in a triple-monochromator configuration and coupled to a cooled CCD detector. A stabilized 785 nm solid-state laser was used for excitation. The backscattered signal was collected through a confocal microscope, producing a lateral laser spot of approximately $1 \text{ }\mu\text{m}$. The instrumental spectral resolution was better than 0.1 cm^{-1} , and the wavenumber axis was calibrated using the 520.7 cm^{-1} line of crystalline silicon.

The incident power was attenuated and kept constant for all specimens to minimize local heating and surface modification; however, the absolute power at the crystal surface was not independently logged. At each surface position, five consecutive 20 s acquisitions were co-added, giving an effective integration time of 100 s , and the condition-level spectrum was obtained by averaging measurements at five spatially separated positions. Only these condition-averaged archived spectra were available for the present reanalysis; the five point-resolved spectra could not be fitted independently. Therefore, the nonlinear-fit standard errors describe the uncertainty of the averaged line-shape model and do not quantify point-to-point or specimen-to-specimen variability. Absolute Raman intensity was not used as a quantitative damage metric.

The spectra were corrected for the instrumental response and processed over 55–485 cm^{-1} . A broad Nd-related fluorescence background was estimated with asymmetric least-squares smoothing [34] by minimizing

$$Q = \sum_i w_i (y_i - z_i)^2 + \lambda \sum_i (\Delta^2 z_i)^2, \quad \lambda = 10^6, |p| = 0.001 \quad (5)$$

The background-subtracted spectra were fitted without numerical smoothing by sums of Lorentzian profiles:

$$I(\omega) = B(\omega) + \sum_j \frac{A_j}{1 + 4 \left[\frac{\omega - \omega_j}{\Gamma_j} \right]^2} \quad (6)$$

where ω_j and Γ_j are the fitted center and FWHM. Because the measurement was not polarization-resolved and the exact sample azimuth was not fixed, the 144/145, 214/215, and 449–470 cm^{-1} regions are treated as effective overlapping envelopes. No fixed Raman probing depth was assigned because the confocal axial response and the wavelength-dependent NdGaO_3 absorption at 785 nm were not independently calibrated. Accordingly, the Raman spectra are interpreted as near-surface-weighted but not quantitatively depth-resolved measurements.

The full 55–485 cm^{-1} spectrum was represented by 11 effective Lorentzian components. In the local diagnostic fits, amplitudes and FWHM values were constrained to positive values, centers were restricted to predefined spectral windows, and a local linear residual background was included. Supplementary Figure S2 and Table S3 report residuals, R^2 , normalized RMSE, center–FWHM parameter correlations, and AsLS baseline sensitivity. Repeating the fits over $\lambda = 5 \times 10^5$ – 2×10^6 and $p = 0.0005$ – 0.002 changed the listed FWHM values by less than 0.002 cm^{-1} . The instrumental resolution ($<0.1 \text{ cm}^{-1}$) is negligible relative to the observed 8–21 cm^{-1} widths and was not deconvolved. These diagnostics remain conditional on the adopted component model and do not restore the unavailable spatially resolved spectra.

The analysis uses a consistent reporting structure: one calibration and acquisition protocol for the full series, a common background treatment, local-window Lorentzian models, explicit residual and covariance diagnostics, a baseline-sensitivity test, and a separate assessment of instrumental broadening. The nominal integration was 100 s at each of five positions, corresponding to 500 s per condition before spatial averaging. Peak centers and FWHM values—not absolute Raman intensity—are therefore the quantitative Raman observables. This workflow supports condition-averaged line-shape comparison but does not provide independent specimen replication.

2.5. UV–Vis–NIR Transmission and Differential Attenuation

Room-temperature transmission spectra were measured with an Agilent Cary 7000 Universal Measurement Spectrophotometer over 190–2000 nm. All specimens had the same nominal thickness of 0.5 mm and were measured in the same orientation. The pristine transmission was converted to absorbance as

$$A(\lambda) = -\log_{10} \left[\frac{T(\lambda)}{100} \right] \quad (7)$$

The radiation-induced differential attenuation was calculated from the transmission ratio and normalized to the SRIM projected range:

$$\Delta\alpha(\lambda, \Phi) = \frac{\ln(T_0/T_\Phi)}{R_p} \quad (8)$$

$$\Delta\alpha(\lambda, \Phi) = \frac{\ln(10)(A_\Phi - A_0)}{R_p}$$

For equal-thickness specimens, the transmission ratio suppresses the common unmodified-bulk and constant-surface contributions to first order. Nevertheless, the measured transmission integrates the complete 0.5 mm optical path, whereas the irradiated zone is approximately 10.95 μm thick. Normalization by R_p therefore defines an effective layer-averaged differential attenuation; if the optically active defect depth is smaller than R_p , the local attenuation coefficient would be larger. Because reflectance and ellipsometric depth profiles were not measured, $\Delta\alpha$ is not a reflectance-corrected absolute absorption coefficient. Unchanged bulk-integrated Nd^{3+} peak positions are not used as direct proof of unchanged local coordination inside the irradiated layer. The Nd^{3+} manifold assignments follow established rare-earth absorption data [35].

2.6. Analytical Uncertainty, Fit Diagnostics, and Evidential Scope

Each condition is represented by one independent specimen. The XRD and Raman profile fits provide model-conditional analytical uncertainties, but no specimen-level standard deviations or inferential confidence intervals can be calculated. No statistical hypothesis tests were performed. Conditional 95% fit intervals, where useful, correspond to ± 1.96 times the reported formal standard errors and must not be interpreted as replicate confidence intervals. At 1×10^{12} ions cm^{-2} , the d_{110} estimate is based on two surviving harmonics and two fitted parameters (d_{110} and a common angular offset), so the model has no residual degrees of freedom. The reported uncertainty is propagated from the individual local peak fits and represents model-conditioned precision rather than independent reproducibility.

The archived Raman files contain condition-level averages of measurements made at five surface positions rather than the five individual point spectra. Consequently, line-center and FWHM errors quantify the nonlinear fit to the averaged spectrum but cannot reconstruct spatial distributions. The unresolved 214/215 cm^{-1} feature is retained only as a descriptive envelope; no mode Grüneisen coefficient or force-constant change is extracted. XRD integrated-intensity errors likewise describe local profile fits and exclude realignment, curvature, footprint, and rocking-curve redistribution. Only one archived optical transmission scan is available for each specimen, so no repeat-scan standard deviation, confidence interval, or specimen-level uncertainty can be assigned to $\Delta\alpha$; the displayed numerical precision is not a statistical measurement uncertainty.

A single-impact track-overlap formalism is available in the literature [36], but it is not applied quantitatively here because the track radius was not measured and only two irradiated fluences were examined. No onset threshold, overlap fraction, or interaction regime is inferred from the present dataset.

The principal conclusions are therefore restricted to a descriptive comparison of the three measured conditions and to observables directly supported by the XRD, Raman, and transmission data.

3. Results

3.1. XRD Phase Retention, Information Depth, and Harmonic Response

Figure 1 summarizes the direction-specific XRD analysis. The full scans retain the (110), (220), and (330) specular sequence expected for the starting (110)-oriented crystal, and no new sharp phase reflection appears after irradiation. Because only one reciprocal-lattice direction was measured, these reflections demonstrate persistence of the oriented parent-phase sequence but do not independently re-establish the complete Pbnm space group. The absolute diffuse background in the 24–36° interval does not show a systematic growth that could be converted into an amorphous fraction. The local windows show

that the lower-fluence specimen has a nearly common positive displacement, whereas the higher-fluence specimen shifts toward smaller angles and loses the high-order signal.

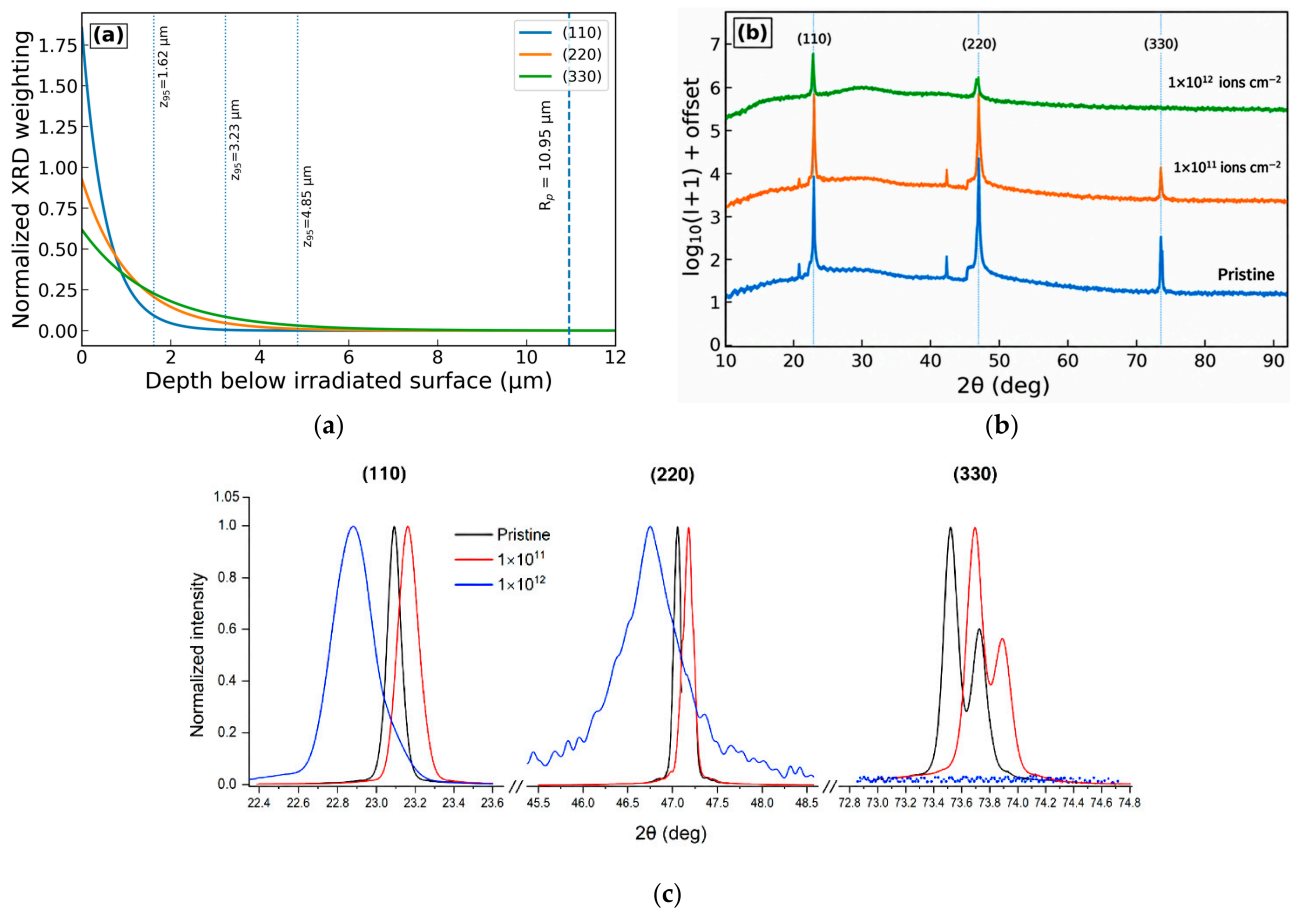


Figure 1. XRD response of NdGaO₃(110): (a) calculated Cu Kα depth weighting and z_{95} values relative to R_p ; (b) complete symmetric scans in logarithmic representation; and (c) narrow local windows of the (110), (220), and (330) reflections plotted on a common normalized offset scale. The 1×10^{12} ions cm⁻² (330) signal is not resolved above the local background.

At 1×10^{11} ions cm⁻², the (110), (220), and (330) peaks shift by $+0.0493^\circ$, $+0.0484^\circ$, and $+0.0455^\circ$. Their near-constant displacement over the angular range is characteristic of a common alignment offset. The joint fit yields $d_{110} = 3.86535 \pm 0.00034$ Å compared with 3.86511 ± 0.00027 Å for pristine, giving $\epsilon_{110} = +0.006 \pm 0.011\%$, which is not distinguishable from zero within the propagated fit uncertainty. At 1×10^{12} ions cm⁻², only the (110) and (220) harmonics remain available; they shift by -0.2119° and -0.3442° . A two-parameter fit to these two reflections gives $d_{110} = 3.88478 \pm 0.00150$ Å and $\epsilon_{110} = +0.509 \pm 0.040\%$. Because the high-fluence fit has zero residual degrees of freedom and no specimen replicate, this value is reported as a model-conditioned estimate rather than an independently reproducible strain measurement.

The supplementary residual analysis supports the adequacy of the local line-shape model within the selected windows, but it does not validate absolute angular accuracy or alignment reproducibility. The 1×10^{12} ions cm⁻² harmonic solution is exactly determined by two reflections and two parameters and is therefore retained only as a model-conditioned point estimate.

The integrated intensity captured in the coupled specular θ - 2θ condition differs strongly among the three specimens. At 1×10^{11} ions cm⁻², the (110), (220), and (330) fitted areas retain $78.10 \pm 10.05\%$, $54.87 \pm 2.62\%$, and $41.02 \pm 1.41\%$ of the pristine val-

ues. At 1×10^{12} ions cm^{-2} , the (110) and (220) values decrease to $9.35 \pm 0.46\%$ and $1.29 \pm 0.06\%$, and (330) is not detected above the local background (Figure 2 and Table 2). The (220) FWHM ratio is 1.08 ± 0.10 times the pristine value at 1×10^{11} ions cm^{-2} and 7.83 ± 0.73 times that of the pristine reflection at 1×10^{12} ions cm^{-2} . These are local-profile fitting errors only. Because no repeated realignment scans, rocking curves, or reciprocal-space maps are available, the large intensity changes cannot be assigned uniquely to loss of long-range coherence; curvature, footprint, mosaic redistribution, and alignment sensitivity may contribute.

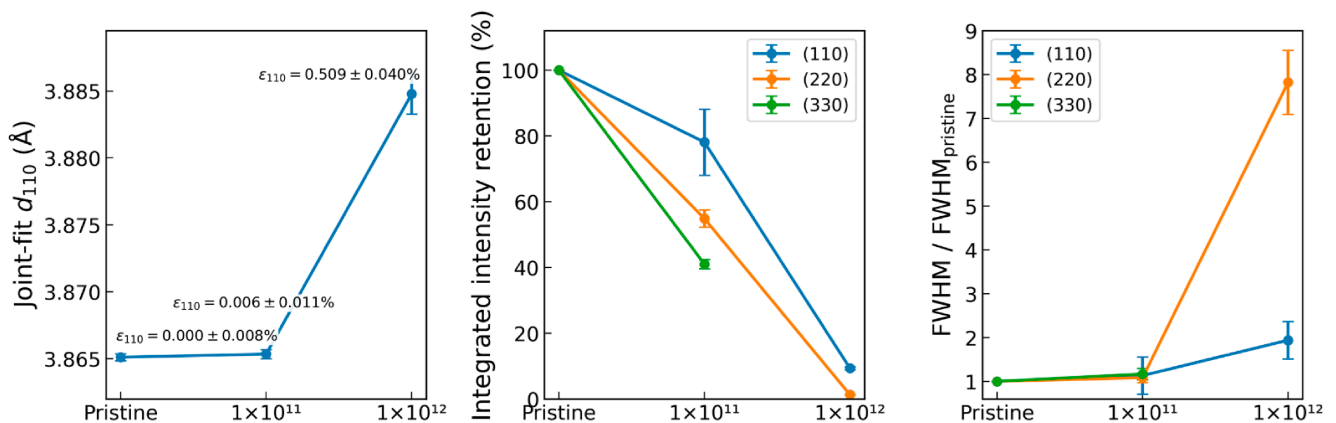


Figure 2. Quantitative XRD evolution of d_{110} and ϵ_{110} , fitted integrated-intensity retention in the coupled θ – 2θ condition, and FWHM ratios relative to pristine. Error bars are propagated 1σ local-profile fitting errors; they do not represent specimen-to-specimen, repeat-alignment, or rocking-curve uncertainties. The 1×10^{12} ions cm^{-2} d_{110} estimate is obtained from two reflections and two model parameters.

Table 2. Quantitative XRD parameters.

Condition	d_{110} (Å)	ϵ_{110} (%)	$I(110)/I_0$ (%)	$I(220)/I_0$ (%)	$I(330)/I_0$ (%)	FWHM(110)/FWHM ₀	FWHM(220)/FWHM ₀
Pristine	3.86511 ± 0.00027	0 (reference)	100 (reference)	100 (reference)	100 (reference)	1.00 (reference)	1.00 (reference)
1×10^{11} ions/ cm^2	3.86535 ± 0.00034	$+0.006 \pm 0.011$	78.10 ± 10.05	54.87 ± 2.62	41.02 ± 1.41	1.13 ± 0.43	1.08 ± 0.10
1×10^{12} ions/ cm^2	3.88478 ± 0.00150	$+0.509 \pm 0.040$	9.35 ± 0.46	1.29 ± 0.06	not detected	1.94 ± 0.43	7.83 ± 0.73

The calculated z_{95} values are all smaller than R_p , so the symmetric XRD signal is dominated by the ion-modified depth interval under the attenuation model. The severe intensity loss is interpreted as suppression of coherent specular scattering by static displacement, a depth-dependent spacing distribution, specimen curvature, and/or mosaic tilt. These contributions are not separated by coupled θ – 2θ scans, and the result is not reported as 90–99% amorphization or as a quantitative mosaic spread.

3.2. Raman Background, Decomposition, and FWHM Evolution

The common background treatment and normalized spectra are shown in Figure 3. A Pbnm-like Raman fingerprint remains recognizable at both fluences, which demonstrates survival of characteristic local vibration groups but does not independently confirm the full space group in the irradiated layer. Broadening is most evident in the low-frequency 144/145 complex, the effective 214/215 band, and the upper 449–470 cm^{-1} envelope.

Figure 4 shows the full-range Lorentzian decomposition for every condition. The individual components are a consistent line-shape representation rather than polarization-

resolved normal modes. Because only condition-averaged archived spectra were available, the fits do not yield a distribution across the five measured positions.

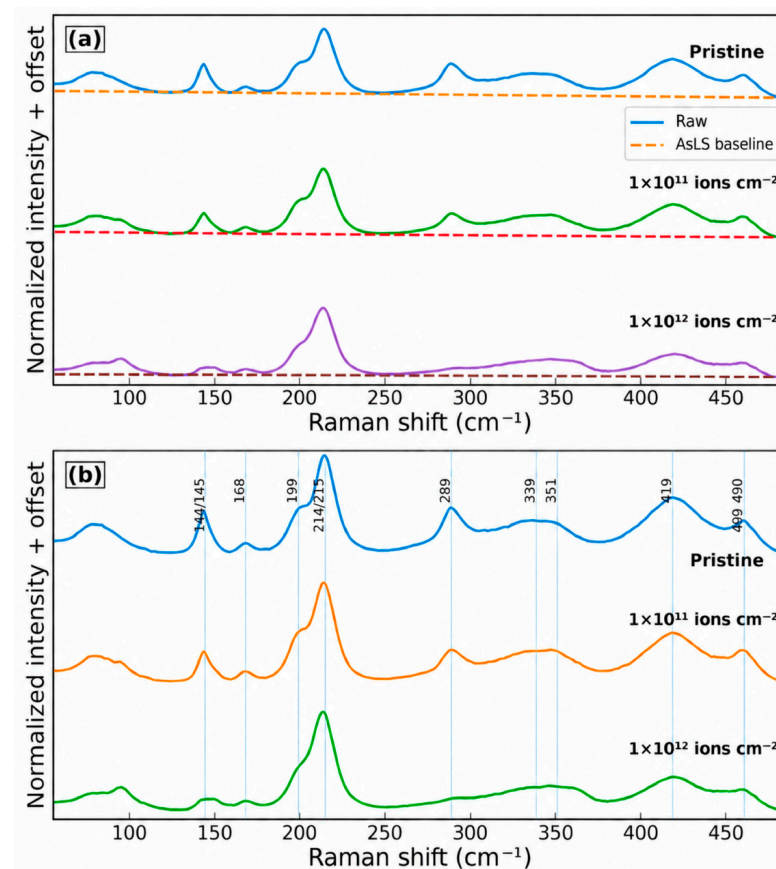


Figure 3. Raman processing: (a) raw spectra and AsLS backgrounds; (b) normalized spectra after background subtraction.

Three effective features show progressively larger fitted FWHM values across the three condition-averaged spectra. The 168 cm^{-1} band changes from 8.02 ± 1.84 to 8.44 ± 1.52 and $9.28 \pm 1.90 \text{ cm}^{-1}$; the $214/215 \text{ cm}^{-1}$ envelope changes from 15.14 ± 0.23 to 16.37 ± 0.24 and $18.08 \pm 0.34 \text{ cm}^{-1}$; and the $449\text{--}470 \text{ cm}^{-1}$ envelope changes from 13.96 ± 0.74 to 15.21 ± 0.72 and $16.02 \pm 1.39 \text{ cm}^{-1}$. The uncertainties are nonlinear-fit standard errors of the averaged spectra, not spatial standard deviations. The fitted $214/215 \text{ cm}^{-1}$ center changes from 214.60 ± 0.04 to 214.16 ± 0.05 and $213.56 \pm 0.06 \text{ cm}^{-1}$. The $144/145$ complex changes strongly, but its overlap sensitivity prevents interpretation as a single-mode linewidth.

For the principal local windows, the residual diagnostics give $R^2 = 0.968\text{--}0.9997$ and normalized RMSE = $0.56\text{--}4.71\%$ (Supplementary Figure S2 and Table S3). The largest covariance and residual structure occur for the high-fluence $144/145 \text{ cm}^{-1}$ complex, reinforcing its treatment as an overlap-sensitive envelope rather than a resolved normal mode.

For the stated line-shape task (Figure 5), the Raman dataset is analytically adequate: the selected observed FWHM values (approximately $8\text{--}21 \text{ cm}^{-1}$) are at least about 80 times larger than the $<0.1 \text{ cm}^{-1}$ instrumental resolution; the tested AsLS parameter range changes the selected FWHM values by less than 0.002 cm^{-1} ; and the residual metrics quantify where the effective-component model performs well and where overlap is strongest. These checks support extraction of condition-averaged centers and FWHM descriptors. They do not establish point-to-point or specimen-to-specimen statistical significance, which remains outside the archived design.

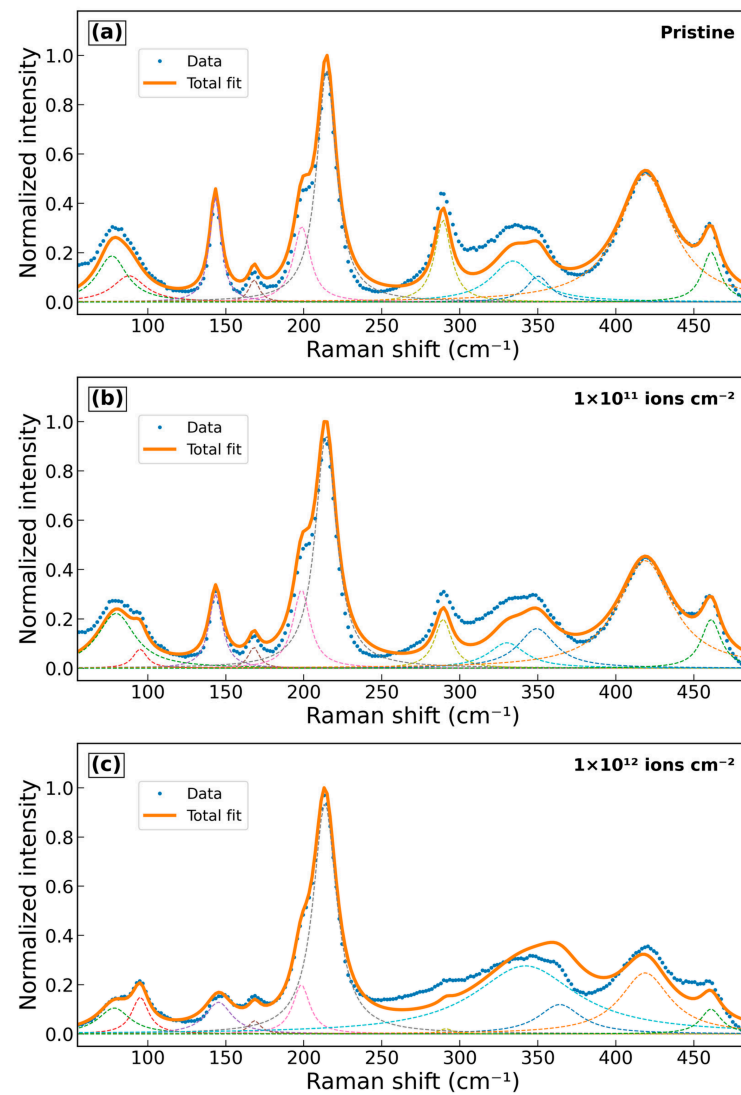


Figure 4. Full-range Lorentzian decomposition of the Raman spectra of NdGaO₃(110) single crystals: (a) pristine sample; (b) sample irradiated with 147 MeV Kr ions at a fluence of 1×10^{11} ions/cm²; and (c) sample irradiated at 1×10^{12} ions/cm². Blue dots represent the experimental, baseline-corrected spectra, while solid orange curves represent the total Lorentzian fits. Thin dashed curves in different colors indicate the individual Lorentzian components contributing to the total fitted spectrum.

Table 3. Raman centers and FWHM values compared with two room-temperature literature datasets.

Band (cm ⁻¹)	Pristine ω /FWHM (cm ⁻¹)	1×10^{11} ω /FWHM (cm ⁻¹)	1×10^{12} ω /FWHM (cm ⁻¹)	Δ FWHM (%)	$\Delta\omega$ (cm ⁻¹)	Kamishima et al. [23] (cm ⁻¹)	Suda et al. [24] (cm ⁻¹)	Assessment
144/145	143.36 ± 0.08 8.88 ± 0.46	143.54 ± 0.10 10.38 ± 0.58	145.39 ± 0.41 20.73 ± 2.49	+133.4	+2.03 ± 0.42	144 B _{2g} ; 145 A _{1g}	144 B _{2g} ; 145 A _{1g}	strong; overlap-sensitive
168 B _{3g}	168.19 ± 0.37 8.02 ± 1.84	167.95 ± 0.30 8.44 ± 1.52	168.46 ± 0.37 9.28 ± 1.90	+15.7	+0.28 ± 0.52	168 B _{3g}	168 B _{3g}	fit trend; large uncertainty
199 B _{3g}	198.78 ± 0.12 13.19 ± 0.60	198.56 ± 0.12 13.42 ± 0.58	198.40 ± 0.23 13.28 ± 1.11	+0.7	−0.38 ± 0.26	199 B _{3g}	199 B _{3g}	no monotonic FWHM trend
214/215	214.60 ± 0.04 15.14 ± 0.23	214.16 ± 0.05 16.37 ± 0.24	213.56 ± 0.06 18.08 ± 0.34	+19.4	−1.04 ± 0.08	214 B _{1g} ; 215 A _{1g}	214 B _{1g} ; 215 A _{1g}	unresolved envelope; descriptive
289/290	289.16 ± 0.12 12.67 ± 0.59	289.32 ± 0.14 13.22 ± 0.68	291.09 ± 0.49 10.00 ± 2.22	−21.1	+1.94 ± 0.51	289 A _{1g}	290 A _{1g}	fit/geometry sensitive
449–470	461.05 ± 0.14 13.96 ± 0.74	461.12 ± 0.14 15.21 ± 0.72	460.96 ± 0.25 16.02 ± 1.39	+14.8	−0.09 ± 0.29	449 B _{1g} ; 463 B _{2g} ; 470 A _{1g}	449 B _{1g} ; 463 B _{2g} ; 470 A _{1g}	effective envelope broadening

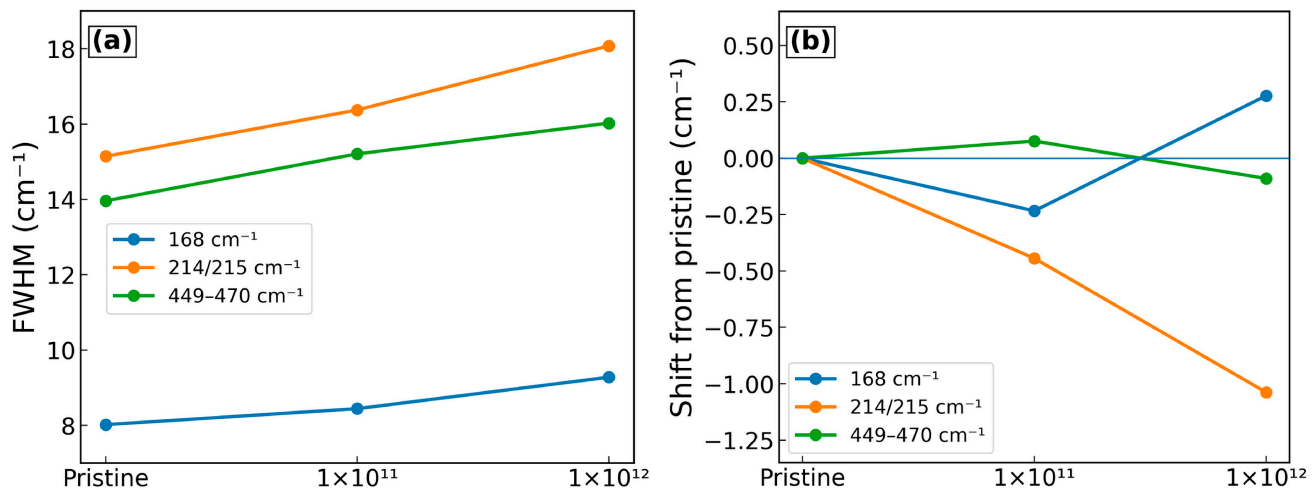


Figure 5. Fluence dependence of (a) fitted Raman FWHM and (b) fitted peak shifts relative to pristine. The symbols describe the three archived condition-averaged spectra; connecting lines are visual guides, not a statistically replicated dose–response fit. Formal uncertainties for the plotted descriptors are given in Table 3. Separate local-refit diagnostics and their conditional intervals are reported in Supplementary Tables S3 and S5 and Figure S2.

All spectral values in Table 3 are in cm^{-1} . Values after $\pm$ are 1σ nonlinear-fit standard errors for the condition-averaged spectra. The literature columns are symmetry-resolved room-temperature frequencies; the present values are effective centers from spectra acquired without polarization analysis. No specimen-level or point-to-point statistical inference is made. Supplementary Tables S3 and S5 report separate local diagnostic refits and their own conditional intervals; their values are not substituted for the descriptors in this table.

3.3. Optical Transmission, Differential Attenuation, and Nd^{3+} Manifolds

The transmission spectra and effective differential attenuation are shown in Figure 6. The pristine crystal has a median transmittance of 73.46% in the 950–1300 nm window. Irradiation produces a weak nearly broadband contribution in the NIR and visible regions and a larger near-UV response. The median $\Delta\alpha$ in the 275–285 nm interval is 224.3 cm^{-1} at $1 \times 10^{11} \text{ ions cm}^{-2}$ and 388.7 cm^{-1} at $1 \times 10^{12} \text{ ions cm}^{-2}$. These values use $R_p = 10.95 \mu\text{m}$ as an operational normalization depth; they are effective layer-averaged differential attenuation coefficients rather than independently depth-resolved local absorption coefficients.

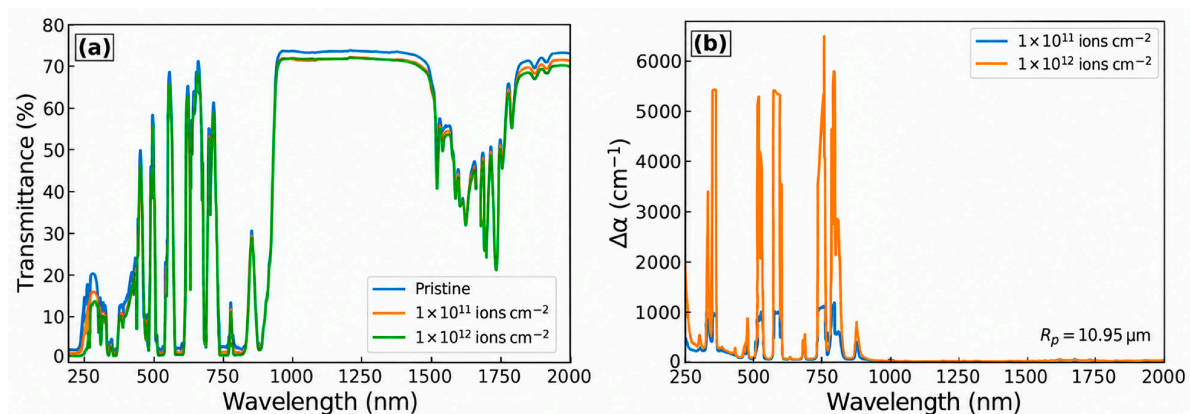


Figure 6. Optical response: (a) measured UV–Vis–NIR transmission; (b) radiation-induced differential attenuation normalized to $R_p = 10.95 \mu\text{m}$.

Thirteen representative Nd^{3+} manifolds are identified in the pristine spectrum (Figure 7 and Tables 4 and 5). For six unsaturated bands, the measured maxima are also reported for the irradiated specimens. The largest sampled difference is 0.5 nm for the 1730 nm band; the other selected maxima are unchanged at the wavelength step used. Because transmission traverses the full 0.5 mm specimen, this stability is a bulk-integrated observation and does not demonstrate unchanged local Nd^{3+} coordination within the approximately 10.95 μm irradiated layer.

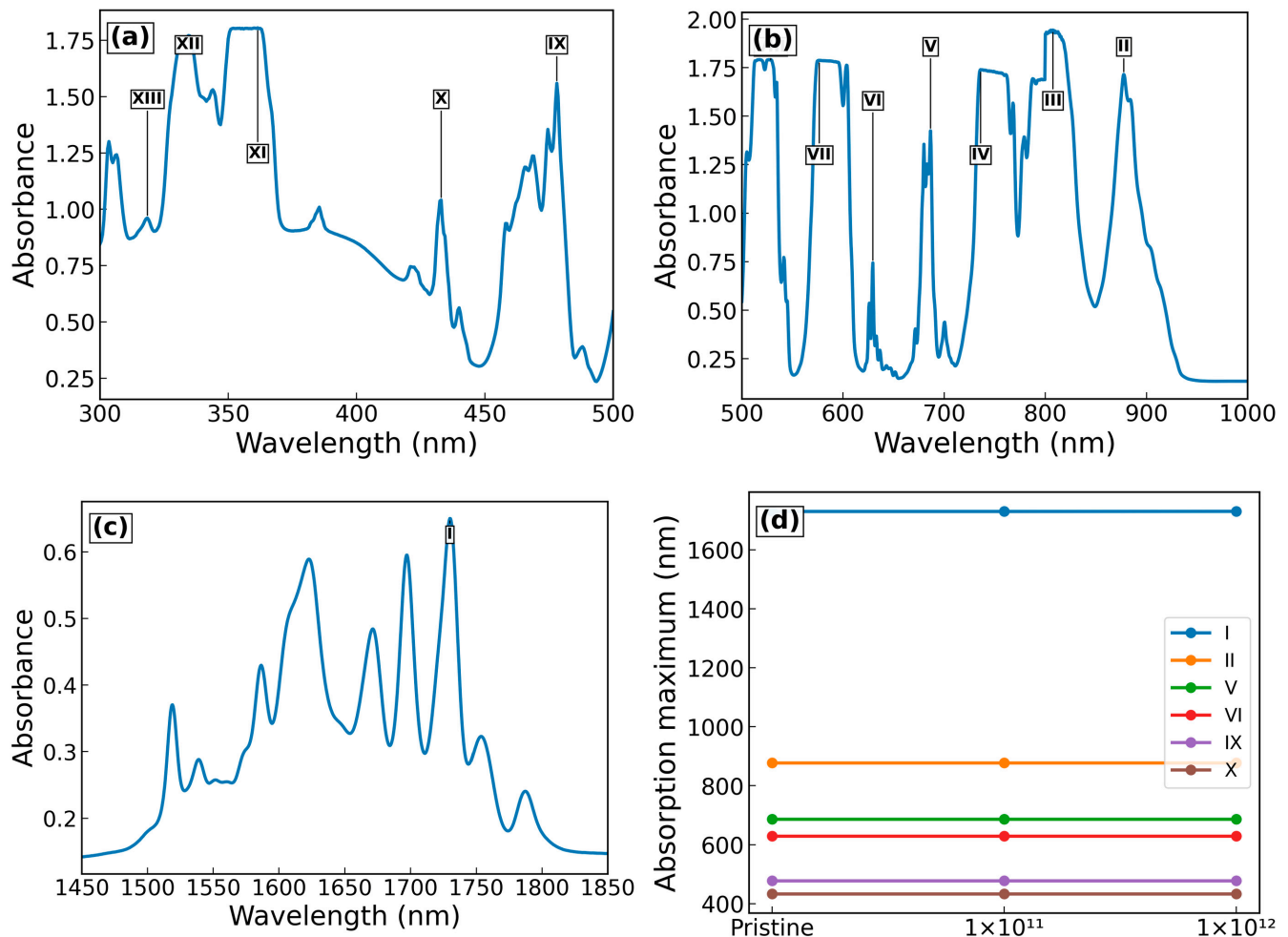


Figure 7. Bulk-integrated Nd^{3+} optical response: pristine absorption manifolds in (a) 300–500 nm, (b) 500–1000 nm, and (c) 1450–1850 nm; (d) measured positions of selected unsaturated maxima. The measurement is not depth selective for the irradiated layer.

Table 4. Representative Nd^{3+} absorption manifolds and measured positions of selected unsaturated bands. “n.e.” denotes not evaluated because of saturation, overlap, or insufficient isolation.

No.	Transition from $^4\text{I}_{9/2}$	λ_0 (nm)	λ_{11} (nm)	λ_{12} (nm)	max $ \Delta\lambda $ (nm)	E_0 (eV)	Assessment
I	$^4\text{I}_{15/2}$	1730.0	1730.0	1730.5	0.5	0.717	NIR Stark manifold
II	$^4\text{F}_{3/2}$	877.5	877.5	877.5	0.0	1.413	unsaturated NIR maximum
III	$^4\text{F}_{5/2} + ^2\text{H}_{9/2}$	807.5	n.e.	n.e.	n.e.	1.535	n.e.; overlapping
IV	$^4\text{F}_{7/2} + ^4\text{S}_{3/2}$	736.0	n.e.	n.e.	n.e.	1.685	n.e.; red/NIR group
V	$^4\text{F}_{9/2}$	686.5	686.5	686.5	0.0	1.806	unsaturated red maximum
VI	$^2\text{H}_{11/2}$	629.5	629.5	629.5	0.0	1.970	unsaturated visible maximum
VII	$^4\text{G}_{5/2} + ^2\text{G}_{7/2}$	576.5	n.e.	n.e.	n.e.	2.151	n.e.; hypersensitive group

Table 4. Cont.

No.	Transition from $^4I_{9/2}$	λ_0 (nm)	λ_{11} (nm)	λ_{12} (nm)	max $ \Delta\lambda $ (nm)	E_0 (eV)	Assessment
VIII	$^4G_{7/2} + ^2G_{9/2} + ^2K_{13/2}$	528.5	n.e.	n.e.	n.e.	2.346	n.e.; overlapping
IX	$^2K_{15/2} / ^2G_{9/2} / ^4G_{11/2}$	478.0	478.0	478.0	0.0	2.594	unsaturated blue maximum
X	$^4P_{1/2} + ^2D_{5/2}$	433.0	433.0	433.0	0.0	2.863	unsaturated blue-violet maximum
XI	high-lying $^4D, ^2I, ^2L$	361.5	n.e.	n.e.	n.e.	3.430	n.e.; UV group
XII	high-lying $4f^3$	334.5	n.e.	n.e.	n.e.	3.707	n.e.; UV group
XIII	$^4D_{7/2} + ^2I_{13/2} + ^2L$	318.5	n.e.	n.e.	n.e.	3.893	n.e.; near-edge group

Table 5. Median transmittance and differential attenuation in selected windows.

Window	Range (nm)	T_0 (%)	T_{11} (%)	T_{12} (%)	$\Delta\alpha_{11}$ (cm $^{-1}$)	$\Delta\alpha_{12}$ (cm $^{-1}$)
NIR transparent	950–1300	73.46	71.78	71.86	21.3	19.9
Visible	645–665	67.74	65.11	65.08	35.3	35.0
Blue	445–455	48.02	44.56	44.65	68.4	65.8
Near-UV	275–285	20.09	15.67	13.13	224.3	388.7

4. Discussion

4.1. Exploratory Comparison of the Three Independently Measured Specimens

The two irradiated specimens show clearly different measured responses, but the design does not establish a continuous fluence dependence, damage threshold, or saturation regime. Because each condition is represented by one independent crystal, the trajectory in Figure 8 is a descriptive comparison of three specimen states and may contain specimen-to-specimen variability. It should not be interpreted as a statistically replicated dose-response curve.

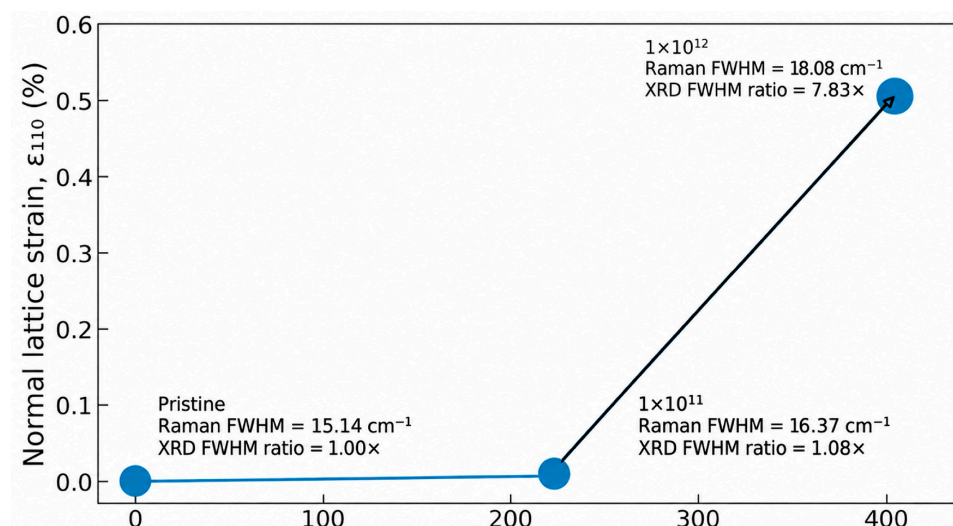


Figure 8. Descriptive comparison in optical–strain space. Marker area is scaled explicitly as $A_m = A_0(\text{FWHM}_{220}/\text{FWHM}_{220,0})$, and the labels give the fitted FWHM of the 214/215 cm $^{-1}$ Raman envelope. Strain error bars are propagated local-profile fit errors rather than specimen-level standard deviations.

At 1×10^{11} ions cm $^{-2}$, the near-UV differential attenuation is 224.3 cm $^{-1}$, whereas $\varepsilon_{110} = +0.006 \pm 0.011\%$ remains unresolved and the (220) FWHM is 1.08 ± 0.10 times the pristine value. The Raman FWHM of the 214/215 cm $^{-1}$ envelope is 16.37 ± 0.24 cm $^{-1}$.

At 1×10^{12} ions cm^{-2} , the estimated ε_{110} is $+0.509 \pm 0.040\%$, the (220) FWHM is 7.83 ± 0.73 times that of the pristine reflection, the Raman FWHM is $18.08 \pm 0.34 \text{ cm}^{-1}$, and $\Delta\alpha$ is 388.7 cm^{-1} . These observations suggest that optical and vibrational changes are measurable in the lower-fluence specimen before a large surface-normal spacing change is resolved, but the single-specimen, two-fluence design does not establish a universal sequence or threshold.

4.2. Qualitative Co-Occurrence of XRD and Raman Changes

The Raman measurements are used for a limited analytical task: comparison of condition-averaged peak centers and FWHM values. The calibrated triple-monochromator system, specified sub- 0.1 cm^{-1} instrumental resolution, 500 s nominal integration per condition, common AsLS treatment, residual analysis, parameter-covariance estimates, and baseline-sensitivity tests support this comparison. Related irradiated-gallate studies are discussed in Section 4.6. These methodological checks do not establish statistical generalizability: five surface positions are spatial subsamples of one crystal, not independent irradiated specimens.

The fitted $214/215 \text{ cm}^{-1}$ envelope shifts by $-1.04 \pm 0.08 \text{ cm}^{-1}$ between the pristine and 1×10^{12} ions cm^{-2} condition-averaged spectra, while the XRD harmonic model gives a positive surface-normal spacing change. These changes occur in the same high-fluence specimen and are qualitatively compatible with lattice softening, but no quantitative coupling coefficient is inferred. The Raman feature contains unresolved B_{1g} and A_{1g} contributions, the complete strain tensor is unavailable, the spectra were averaged before fitting, and the absolute laser power was not logged. Accordingly, no mode Grüneisen parameter or force-constant change is reported.

4.3. Crystallochemical Interpretation of the GaO_6 Response

The low-frequency Raman spectrum is sensitive to collective octahedral tilting, bending, and Nd/O displacements. The $\approx 339 \text{ cm}^{-1}$ A_{1g} mode is associated mainly with oxygen-cage rotation or libration, whereas the $449\text{--}470 \text{ cm}^{-1}$ group contains a stronger Ga–O stretching contribution (Figure 9) [23–25]. The conceptual mode classes are summarized in Figure 9. The simultaneous broadening of low- and high-frequency regions indicates a distribution of Ga–O–Ga angles and local Ga–O force constants rather than one uniform bond elongation.

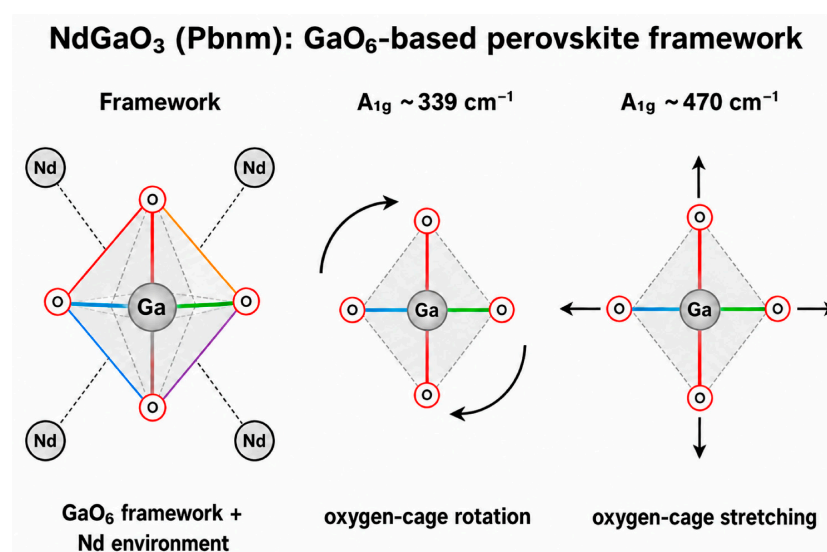


Figure 9. Conceptual vibration classes of the connected GaO_6 framework used for the cautious interpretation of the Raman line-shape changes, based on the mode assignments in Refs. [23–25].

4.4. Suppressed Coherent Diffraction Versus Retained Local Order

The large reduction of the integrated intensity captured in the coupled θ – 2θ condition compared with the moderate Raman FWHM change is not intrinsically contradictory. Symmetric XRD requires long-range registry and angular acceptance across the illuminated area, whereas Raman scattering is governed by local polarizability fluctuations. Static atomic displacements, a depth-dependent d-spacing distribution, curvature, footprint changes, and mosaic redistribution can all reduce or redistribute specular intensity. Without repeated realignment scans, rocking curves, reciprocal-space maps, or cross-sectional microscopy, their contributions cannot be separated, and the intensity decrease cannot be converted uniquely into a loss of crystalline volume or long-range coherence. The surviving Raman groups demonstrate characteristic local vibrational order, but neither Raman nor the restricted collinear XRD series independently confirms the complete Pbnm symmetry of the modified layer.

4.5. Optical Coloration and the Stability of Nd^{3+}

The near-UV growth of the effective differential attenuation is compatible with additional sub-edge electronic states in the ion-modified region. Oxygen vacancies, trapped carriers, vacancy–polaron complexes, and related oxygen-sublattice disorder are plausible hypotheses rather than experimentally identified defects. Because the optical beam traverses the complete 0.5 mm specimen, the damage profile is nonuniform, and reflectance and interference changes were not measured, the R_p -normalized quantity is a model-dependent effective attenuation rather than a material absorption coefficient. If the optically active depth differs from R_p , the local coefficient changes inversely with the assumed depth. The stable bulk-integrated 4f–4f peak positions show only that no shift is resolved in the total transmission spectrum; they do not demonstrate unchanged local coordination within the irradiated layer.

4.6. Comparison with Other Irradiated Complex Oxides

The NdGaO_3 response is consistent with the broader observation that preservation of a Raman fingerprint does not preclude severe structural disorder. In CeO_2 , a fluorite Raman mode can survive while intensity decreases and defect-related broadening develops (Table 6) [37]. Garnet studies show a material-dependent route from amorphization-prone YIG to more disorder-tolerant GGG [38], while a broad Raman survey of irradiated ceramics emphasizes that linewidth and disorder-band changes are host dependent [39]. Composition-dependent pyrochlores similarly demonstrate that short-range order and defect recovery depend on framework chemistry [40]. Independent work on the orthorhombic perovskites LaAlO_3 and YAlO_3 further shows that the balance between nuclear-collision damage and electronic-excitation recovery is strongly composition dependent, providing a non-gallate perovskite benchmark for the present interpretation (Table 6) [41].

Related gallate studies provide the closest benchmarks. GGG irradiated with 147 MeV Kr ions shows structural, optical, and mechanical changes at higher fluences [42]. Two peer-reviewed Crystals articles by an overlapping author team applied closely related high-resolution Raman acquisition, background-corrected spectra, and mode-specific peak/FWHM analysis to 231 MeV Xe- and 147 MeV Kr-irradiated GGG [43,44]. Their relevance here is methodological: they document that this spectroscopy and line-shape workflow is established for swift-heavy-ion-irradiated gallate single crystals, while not replacing the missing independent NdGaO_3 specimen replicates. BaFBr demonstrates that absorption, Raman, and luminescence can evolve non-equivalently under fast Kr irradiation [45]. MgO and BeO studies (Table 6) connect radiation-induced optical loss and strain with vacancy-related defects [46,47], while depth-resolved spinel measurements reveal that

elastic response can vary across the ion range [48]. Raman and diffraction studies of ZnO and Al₂O₃ further show that stress and defect signatures may coexist with retained crystalline order [49,50]. Color-center work in oxide and fluoride crystals confirms that optical spectroscopy can be more sensitive to defect charge states than average diffraction [51–55].

Table 6. Comparison with selected swift-heavy-ion studies.

Material	Irradiation/Probe	Main Response	Relation to NdGaO ₃	Ref.
CeO ₂	SHI; Raman	mode retained; intensity loss and broadening	severe local disorder without required full amorphization	[37]
YIG/GGG	SHI; optical/Raman	different amorphization susceptibility	framework topology controls response	[38]
Ceramic survey	SHI; Raman	host-dependent disorder markers	supports mode-selective interpretation	[39]
Pyrochlores	electronic stopping; XRD/Raman	composition-dependent short-range order	chemistry changes recovery pathway	[40]
GGG	147 MeV Kr; multimodal	strain, optical and mechanical evolution	closest gallate benchmark	[42]
GGG	Xe/Kr; Raman/luminescence	mode retention with broadening	similar local-order persistence	[43,44]
BaFBr	fast Kr; optical/Raman	non-equivalent probe response	supports multimodal analysis	[45]
MgO/BeO	heavy ions; optical/strain	vacancy and residual-stress effects	comparison for coloration and expansion	[46,47]
Spinel	710 MeV Bi; depth-resolved	depth-dependent elastic response	highlights damage gradients	[48]
ZnO/Al ₂ O ₃	SHI; Raman/XRD	stress/defects with retained order	separates defect signatures from phase identity	[49,50]
Oxide/fluoride centers	irradiation; optical	charge-state-dependent color centers	microscopic assignment requires independent evidence	[51]
LaAlO ₃ /YAlO ₃	nuclear collisions and electronic excitation; structural damage	composition-dependent damage thresholds and recovery	independent orthorhombic-perovskite benchmark	[41]

4.7. Integrated Multiscale Response and Methodological Limits

Figure 10 normalizes the main experimental observables to their maximum response. At 1×10^{11} ions cm^{−2}, the optical and Raman changes are already measurable while ϵ_{110} remains unresolved. At 1×10^{12} ions cm^{−2}, the dominant change is the loss and broadening of coherent diffraction, accompanied by local phonon disorder and strong near-UV attenuation. The Nd³⁺ peak positions remain the least sensitive observable.

To compare heterogeneous observables with different dimensions, each parameter was converted to a row-wise response $R_i(\Phi) = |X_i(\Phi) - X_i(0)| / \max_{\Phi} |X_i(\Phi) - X_i(0)|$. The heatmap therefore reports the fraction of the largest change observed within this three-condition dataset and does not compare absolute magnitudes between different physical quantities. A logarithmic color normalization was used only to make weak nonzero responses visible: numerical zeros are exact zeros in the annotations and are mapped to the lower color limit for display, whereas pale nonzero cells represent small but finite normalized responses.

Fluence-dependent structural, vibrational, and optical responses

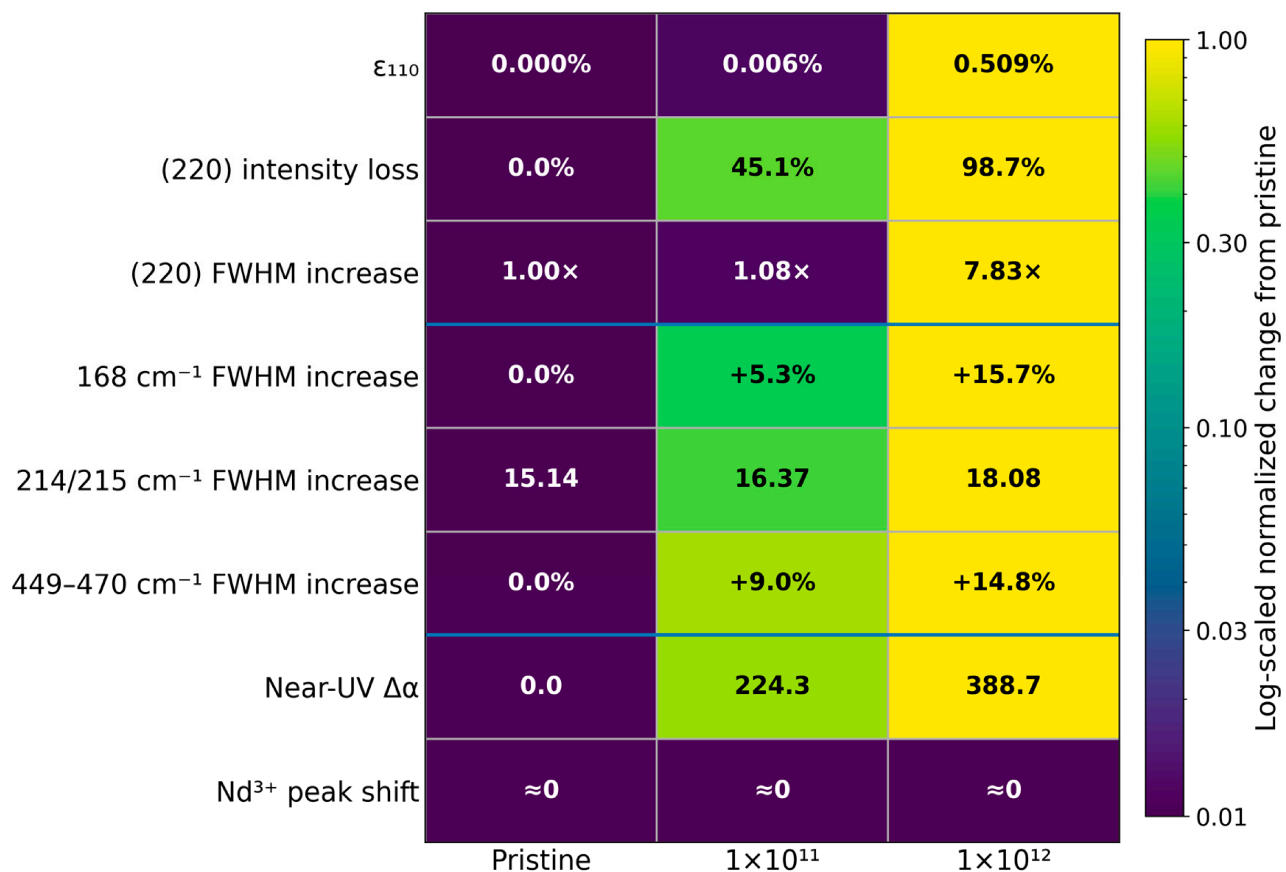


Figure 10. Cross-method heatmap of the three measured NdGaO₃(110) conditions. Colors represent the logarithmically scaled, row-wise normalized change from pristine, and numerical annotations report the measured values. An annotated zero denotes an exact zero by definition or within the adopted descriptor and is plotted at the lower color limit; pale nonzero cells represent small but finite responses.

Figure 11 separates directly measured or model-derived quantities from a non-unique microscopic hypothesis. Dominant electronic stopping and the SRIM range are model inputs. Dense electronic excitation, transient lattice heating, oxygen/electronic defect production, and interaction of local strain fields are plausible processes drawn from the swift-heavy-ion literature, but none was directly measured in this experiment. The experimentally established observations are limited to the direction-specific XRD response, condition-averaged Raman line shapes, and bulk-integrated transmission. The figure must therefore be read as one scenario consistent with the data, not as a demonstrated reaction pathway.

The principal limitations are one independent specimen per condition and no paired before/after measurements; only two irradiated fluences; no run-specific estimate of absolute fluence uncertainty, independent beam-uniformity map, or time-resolved current record; and no in situ specimen-temperature monitoring. The flux and exposure times in Section 2.1 are calculated nominal quantities, and the scanning frequencies and uniformity are standard system characteristics. Additional limitations are the one-direction symmetric XRD geometry; the absence of an external angular standard and repeat realignment scans; the two-reflection/two-parameter high-fluence strain fit; the absence of rocking curves, reciprocal-space maps, asymmetric reflections, and cross-sectional microscopy; Raman fitting of archived five-position averages rather than point-resolved spectra; the lack of calibrated Raman sampling depth and absolute laser power; and one bulk-transmission

spectrum per specimen without depth profiling or reflectance. Accordingly, no specimen-level statistics, repeat-scan optical uncertainty, quantitative mosaicity, damage threshold, track radius, complete space-group retention, defect charge state, or unique microscopic mechanism is claimed.

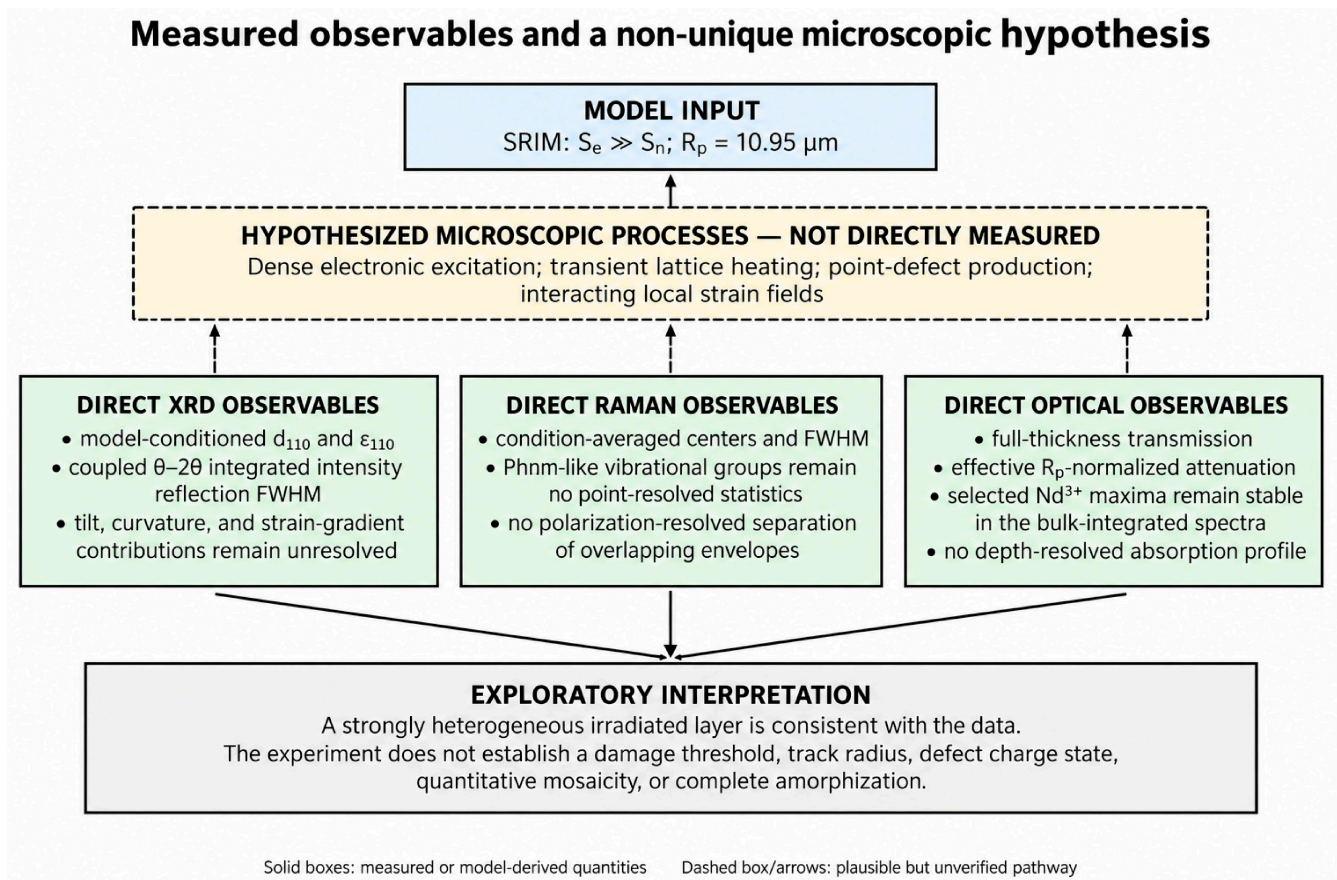


Figure 11. Directly measured/model-derived observables and a non-unique microscopic hypothesis consistent with the available data. Solid boxes summarize measurements or SRIM-derived inputs; the dashed box and arrows identify plausible processes that were not directly observed.

5. Conclusions

- The (110), (220), and (330) specular sequence of the starting orthorhombic crystal remains identifiable after irradiation, and no secondary crystalline phase is detected; the restricted symmetric geometry does not independently confirm the complete Pbnm space group in the modified layer.
- For the single specimen irradiated to $1 \times 10^{11} \text{ ions cm}^{-2}$, the approximately constant $+0.046$ – $+0.049^\circ$ shift is dominated by a common angular offset, and $\epsilon_{110} = +0.006 \pm 0.011\%$ is not distinguishable from zero within the propagated fit uncertainty.
- For the single specimen irradiated to $1 \times 10^{12} \text{ ions cm}^{-2}$, the two-harmonic model gives $d_{110} = 3.88478 \pm 0.00150 \text{ \AA}$ and $\epsilon_{110} = +0.509 \pm 0.040\%$. In the coupled θ – 2θ condition, the fitted (110) and (220) areas retain $9.35 \pm 0.46\%$ and $1.29 \pm 0.06\%$, and the (220) FWHM is 7.83 ± 0.73 times that of the pristine reflection. These values are model- and alignment-conditional and do not quantify crystalline volume loss or mosaicity.
- The condition-averaged Raman spectra show larger fitted FWHM values for the 168, 214/215, and 449 – 470 cm^{-1} features and a $-1.04 \pm 0.08 \text{ cm}^{-1}$ shift of the unresolved 214/215 cm^{-1} envelope. Calibration, spectral resolution, residual diagnostics, covari-

ance estimates, and baseline-sensitivity testing support these quantities as analytical line-shape descriptors; they remain neither spatial nor specimen-level statistics.

- The selected Nd^{3+} absorption maxima remain stable in the bulk-integrated transmission spectra within the wavelength sampling, while the effective differential attenuation in the 275–285 nm interval reaches 388.7 cm^{-1} at $1 \times 10^{12} \text{ ions cm}^{-2}$; this stability does not establish unchanged local coordination within the irradiated layer.
- The combined observations are consistent with a strained and diffraction-heterogeneous crystalline layer. Complete amorphization, quantitative mosaicity, full space-group retention, a damage threshold, track dimensions, a specific defect charge state, and a unique microscopic pathway are not established. The irradiation operating conditions have been clarified, but one specimen was studied per condition, specimen heating was not monitored, and independent alignment and specimen-reproducibility measurements were unavailable. The conclusions therefore remain exploratory and require independent replication.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/app162010130/s1>, Figure S1, local XRD profile fits and residuals; Table S1, XRD local-fit diagnostics; Table S2, joint harmonic-fit diagnostics; Figure S2, Raman local fits and residuals; Table S3, Raman residual, parameter-correlation, and baseline-sensitivity diagnostics; Tables S4 and S5, conditional XRD and Raman fit intervals; and Table S6, analytical adequacy, methodological precedent, and inferential limits of the Raman workflow.

Author Contributions: Conceptualization, Z.T.K. and A.I.P.; methodology, Z.T.K. and M.K.; software, M.S.T. and M.K.; validation, Z.T.K., M.S.T., E.B.Z., M.K., T.A.S., V.B., and A.I.P.; formal analysis, Z.T.K., A.B., M.K., and A.M.Z.; investigation, Z.T.K., M.K., E.B.Z., T.A.S., V.B., and A.I.P.; resources, T.A.S., V.B., and A.I.P.; data curation, A.B., A.M.Z. and E.B.Z.; writing—original draft preparation, Z.T.K. and M.S.T.; writing—review and editing, all authors; visualization, Z.T.K., A.M.Z., and M.S.T.; supervision, Z.T.K. and A.I.P.; project administration, Z.T.K. and A.I.P.; funding acquisition, Z.T.K. and A.I.P. All authors have read and agreed to the published version of the manuscript.

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Abbreviations

Abbreviation	Definition
AsLS	asymmetric least-squares baseline
CCD	charge-coupled device
FWHM	full width at half maximum
RIA	radiation-induced attenuation
SHI	swift heavy ion

SRIM	Stopping and Range of Ions in Matter
XRD	X-ray diffraction

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