

Subsurface Driven Size-Dependent Elasticity in Nanodiamond

Jiaqi Zhang^{1,2,3}, Chunmeng Liu¹, Xing Li¹, Dongyang Wang¹, Keke Zhao¹, Houlin Ji¹, Yoshifumi Oshima³, Shaobo Cheng^{1,2,*} and Chongxin Shan^{1,†}

¹Henan Key Laboratory of Diamond Materials and Devices, Key Laboratory of Materials Physics, Ministry of Education, and School of Physics, Zhengzhou University, Zhengzhou 450052, China

²Institute of Quantum Materials and Physics, Henan Academy of Sciences, Zhengzhou 450046, China

³School of Materials Science, Japan Advanced Institute of Science and Technology, Nomi, Ishikawa 923-1292, Japan



(Received 4 September 2025; revised 30 January 2026; accepted 16 March 2026; published 10 April 2026)

Diamond, an archetype of hardness and brittleness, can nonetheless display striking elastic compliance at the nanoscale, in sharp contrast to its ultrastiff, fracture prone bulk behavior. Despite recent experimental progress, the atomic scale origin of this anomalous elasticity remains unresolved. Here, we uncover a pronounced size- dependent softening in nanodiamond, with the effective axial Young's modulus decreasing from about 1000 to about 700 GPa as the particle diameter shrinks from 13 to 4 nm. By integrating *in situ* transmission electron microscopy nanomechanical testing with first principles calculations and molecular dynamics simulations, we show that this stiffness reduction does not arise from the surface atomic layers, which remain comparatively stiff, but instead from weakened bonding in a distinct interfacial region between the surface and the crystalline core. These under-coordinated regions localize strain and accommodate large elastic deformation. The results uncover a previously overlooked interfacial mechanism that governs elasticity in brittle nanomaterials and offer design principles for nanomechanical resonators, quantum devices, and thermal transport applications with tunable stiffness.

DOI: [10.1103/b3h5-34wt](https://doi.org/10.1103/b3h5-34wt)

Subject Areas: Condensed Matter Physics,
Materials Science, Mechanics

I. INTRODUCTION

Diamond has long been regarded as the ultimate symbol of hardness and brittleness—an ultrastiff material that is typically fracture prone in bulk. Its unparalleled mechanical strength, superior thermal conductivity, and chemical inertness have secured its place in applications demanding extreme durability, from cutting tools to quantum technologies [1–4]. Traditionally, diamond's exceptional hardness has been viewed as inevitably coupled with extreme brittleness, with catastrophic fracture occurring immediately upon surpassing its elastic limit [5,6]. However, this long-standing perception has been increasingly challenged in recent years. Emerging experimental studies have revealed that when scaled down to nanometer dimensions, diamond can exhibit remarkable elasticity, sustaining large, reversible strains well beyond those achievable in bulk form [7–9]. These observations raise

a central mechanistic question: in ultrasmall nanodiamonds, which atomic-scale motifs govern the effective stiffness and the onset of dissipation under contact loading? Despite this progress, a clear microscopic understanding remains incomplete, and the elastic and failure responses of nanodiamonds—together with the roles of specific atomic-scale structural features—have yet to be systematically established.

One commonly proposed explanation attributes this unusual behavior to the nanoscale dimensions of the diamond particles, which significantly reduce the likelihood of internal defects compared to micro- and macroscale specimens. More importantly, surface effects have been identified as critical factors governing the mechanical response of nanomaterials. At such small length scales, surface atoms exhibit under-coordination and reconstruction phenomena, substantially altering local bonding configurations and mechanical properties [8–10]. It has been suggested that the atomic flatness and improved surface quality of nanodiamonds make it more difficult to initiate surface cracks, thus enhancing their elastic resilience by impeding crack nucleation from surface defects. Furthermore, plastic deformation has been directly observed in diamond structures down to several hundred nanometers in size [11]. While these insights have advanced our understanding, they remain insufficient to fully capture the complex

*Contact author: chengshaobo@zzu.edu.cn

†Contact author: cxshan@zzu.edu.cn

Published by the American Physical Society under the terms of the [Creative Commons Attribution 4.0 International](https://creativecommons.org/licenses/by/4.0/) license. Further distribution of this work must maintain attribution to the author(s) and the published article's title, journal citation, and DOI.

atomic-scale mechanisms governing the mechanical properties of ultrasmall nanodiamonds.

Young's modulus is a key quantity in this context because it directly quantifies stiffness and governs elastic response under applied stress [12,13]. Bulk diamond exhibits an exceptionally high Young's modulus of ~ 1140 GPa [14,15]. As the characteristic size decreases to the nanoscale, however, theory predicts that Young's modulus can deviate from the bulk value due to pronounced size effects, including the increasing surface-to-volume ratio, surface reconstruction, and quantum-confinement-related changes in bonding [16–21]. The sign and origin of these deviations remain debated: some models predict surface-induced stiffening driven by electron redistribution, whereas others predict reduced near-surface stiffness associated with lower coordination at the surface [22–24]. These competing mechanisms inevitably affect the mechanical behavior of nanomaterials. Although size-dependent elasticity is widely reported across nanoscale materials, diamond represents an extreme and technologically central limit where near-bulk stiffness is often anticipated in defect-scarce nanocrystals. Resolving the microscopic origin of any systematic softening in the few-nanometer regime is therefore particularly important. Accordingly, it is crucial to experimentally elucidate their respective contributions at the atomic scale, particularly to achieve a comprehensive understanding of the mechanical properties of nanodiamonds.

Despite extensive theoretical efforts, conclusive experimental evidence remains scarce, and the topic continues to be actively investigated. In recent years, computational studies have increasingly focused on the mechanical properties of ultrasmall nanodiamonds (with diameters below 10 nm). For example, Jiang *et al.* employed first-principles simulations on nanodiamonds with diameters ranging from 0.71 to 1.4 nm, revealing that their Young's modulus was lower than that of bulk diamond and increased with particle size, primarily due to the prevalence of low-coordination surface atoms [25]. In contrast, Tanskanen *et al.* reported that the Young's modulus of diamond nanowires increases as their diameter decreases, attributing this behavior to the redistribution of stress among a larger number of C–C bonds. Although these theoretical perspectives remain controversial, direct experimental validation is still limited, primarily due to the technical challenges involved in characterizing mechanical properties at such small length scales.

To date, most experimental studies have concentrated on nanocrystalline diamond films, typically reporting Young's modulus values comparable to that of bulk diamond [14]. For example, it has been shown that nanocrystalline diamond films with thicknesses below 150 nm can achieve Young's modulus values approaching those of single-crystal diamond when grown under optimized conditions [26]. In addition, Dang *et al.* reported that focused ion beam

(FIB)-processed nanodiamonds with diameters around 200 nm exhibit a Young's modulus of approximately 865 GPa, slightly lower than the theoretical bulk value, likely due to the presence of a surface amorphous carbon layer and growth-induced imperfections [7]. However, the mechanical behavior of ultrasmall, individual nanodiamonds remains poorly explored, and their size-dependent elastic properties have yet to be systematically investigated. This may provide key clues for a systematic understanding of the mechanical properties of nanoscale diamonds.

In this study, we experimentally demonstrate the size-dependent effective axial Young's modulus of nanodiamond through *in situ* mechanical testing performed inside a transmission electron microscope (TEM) at room temperature. Our results reveal that the effective axial Young's modulus of nanodiamonds decreases from about 1000 to about 700 GPa as the diameter decreases. These findings indicate that the Young's modulus of the near-surface region is substantially lower than that of the particle core, confirming that reduced elastic modulus of the near-surface region plays a dominant role in governing the elastic behavior of nanodiamonds at the nanoscale.

II. RESULTS

Figure 1(a) illustrates a schematic of the experimental setup used to measure the mechanical properties of

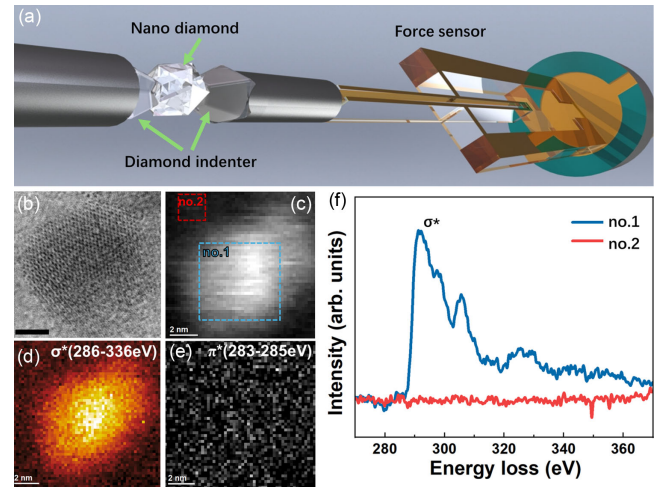


FIG. 1. Measurement system and sample characterization. (a) Schematic illustration of the experimental setup. Nanodiamonds are clamped between two diamond indenters. One is fixed to a quartz LER and another one is fixed to the holder frame. (b) STEM-ABF image of a nanodiamond, scale bar is 2 nm. (c) EELS spectra image of the diamond NPs. (d) EELS mapping image showing the signal between 286–336 eV induced by σ^* orbitals due to sp^3 bonding and (e) signal 283–285 eV induced by transitions to the π^* orbital due to the presence of sp^2 bonding. (f) EELS spectra of the 2 regions containing nanodiamond and the substrate. The absence of sp^2 signal confirms the sp^3 purity of the nanodiamonds.

nanodiamond, a system previously demonstrated to provide high precision and stability in mechanical characterization [18,27–29]. The diamond nanoparticles (NPs) were clamped between two diamond indenters: one attached to the edge of a length-extension resonator (LER; 3EXW-1073, STATEK) and the other fixed to a counterelectrode. The LER-side indenter position was controlled by a tube piezo actuator. Prior to testing, samples were baked at $\sim 100^\circ\text{C}$ for at least 24 h under vacuum to reduce volatile surface contaminants and, as much as possible, to suppress the formation of surface terminal groups. All nanodiamonds were taken from the same batch and prepared using an identical protocol; therefore, E_{surface} should be interpreted as an effective parameter for the specific surface state in our measurements. All experiments were conducted inside a JEM-2000VF TEM (operating at 200 kV) under ultrahigh vacuum conditions (10^{-7} Pa) to minimize contamination and gas adsorption. To assess potential beam-dose and time-dependent effects in *in situ* TEM testing, we additionally conducted control measurements with the electron beam blanked throughout the loading-unloading cycle and compared them with the imaging condition at 80 kV (Figs. S7, S8 [33]).

To evaluate the mechanical response of the nanodiamonds, the LER prong was driven to oscillate at its resonant frequency with a constant amplitude of 15 pm by applying an AC excitation voltage through a phase-locked loop and an oscillation controller (OC4, SPECS). To assess potential amplitude-related hysteresis or feedback artifacts, selected measurements were repeated at a larger oscillation amplitude of 30 pm, yielding consistent dissipation-free elastic ranges, dissipation onset strains, and extracted stiffness or modulus within experimental scatter. The stiffness of the nanodiamond was measured using a frequency modulation technique, a highly sensitive method widely employed in atomic force microscopy (AFM) for detecting force responses. [30–32]. Plastic deformation was identified by tracking the energy dissipation of the resonator, which reflects the energy consumed during irreversible deformation, consistent with prior work [31]. Notably, fluctuations in the measurement signals caused by feedback control and environmental noise did not affect the overall measurement trends or the conclusions drawn from them.

Figure 1(b) presents a high-resolution scanning transmission electron microscopy annular bright-field (STEM-ABF) image of a nanodiamond, clearly displaying the characteristic lattice structure of diamond, thereby confirming its excellent crystallinity. The corresponding electron energy loss spectroscopy (EELS) spectra and mapping data are shown in Figs. 1(c)–1(f). The EELS spectrum of the nanodiamond [Fig. 1(f)] displays distinct features characteristic of diamond, with no detectable sp^2 carbon signal (typically appearing at 284 eV). EELS mapping [Figs. 1(c)–1(e)] further confirms the exclusive presence of sp^3 -hybridized carbon in the nanodiamonds, with no

detectable sp^2 carbon signals either within the particles or in the surrounding area. Additional structural characterization using x-ray diffraction (XRD) and Raman spectroscopy (see Fig. S1 and S2 in Supplemental Material [33]) also verifies the high crystalline quality of the diamond NPs.

To comprehensively investigate the elastic properties of nanodiamonds, individual nanodiamonds were clamped and compressed between diamond indenters, as illustrated in Fig. 2 and Figs. S3–S5 in [33]. Figures 2(a)–2(f) present a representative example of the evolution of both stiffness and energy dissipation during constant-speed compression. From the TEM observations, the nanodiamond was aligned along the $\langle 110 \rangle$ zone axis and compressed along the $\langle 111 \rangle$ direction [Fig. 2(g)]. The nanodiamond used in this measurement had a diameter of 7.3 nm [Fig. 2(a)]. At the onset of loading, the measured stiffness rises rapidly as the contacts are formed. This early increase is quantitatively consistent with classical elastic contact mechanics: the stiffness follows the expected scaling for Hertzian sphere-flat contact. Within our experimental resolution, the stiffness approaches zero as the indentation tends to zero, indicating that an adhesion-dominated JKR-type finite-stiffness offset at zero load is not required under our conditions (Supplemental Material Fig. S6 [33]). These observations highlight the remarkable elastic deformability of nanodiamonds, which sustain unusually large elastic strains. In the initial loading stage, the dissipated energy remains at the baseline level, confirming that the deformation is essentially dissipation-free and elastic.

As the nanodiamond was compressed to about 6.2 nm [Fig. 2(c)], corresponding to a strain of approximately 15%, the dissipated energy increased to ~ 0.05 eV per oscillation

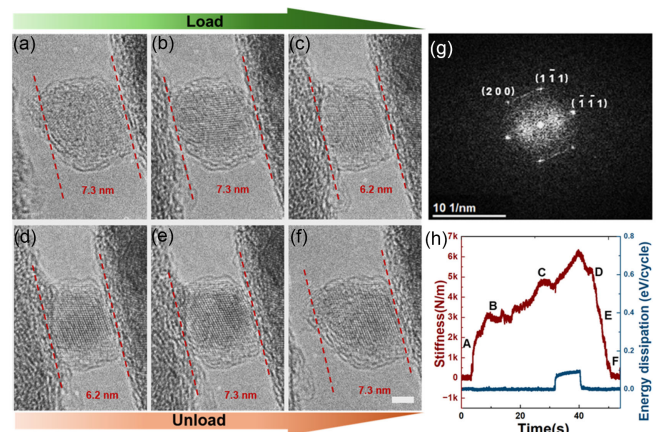


FIG. 2. Measurement of the mechanical properties of the nanodiamond. (a)–(f) TEM images of the nanodiamond during the compression process, the scale bar is 3 nm. (g) The fast Fourier transform (FFT) of the nanodiamond, showing the nanodiamond is compressed along the $\langle 111 \rangle$ direction. (h) Typical evolution of the stiffness and energy dissipation during compression of the nanodiamond.

cycle and subsequently plateaued, indicating the onset of plastic deformation [7,33]. Upon detecting plasticity, the applied load was released, completing the measurement [Fig. 2(d)]. Postcompression TEM images revealed that the nanoparticle retained a comparable lateral size (~ 7.2 nm) along the compression axis, without visible cracking or catastrophic damage. Here “plasticity” refers to a permanent residual strain after full unloading, which we corroborate by same-particle repeat load-unload cycles (elastic overlap vs post-onset irreversible change); the load-unload loops, residual-strain quantification, and dissipation analyses are provided in the Supplemental Material (Fig. S9) [33]. Such plasticity corresponds to atomic rearrangement and amorphization. The observed irreversibility is consistent with atomic rearrangement and local amorphization, supporting a picture in which the elastic-plastic transition in ultrasmall nanodiamonds is governed by strain-induced atomic-scale disordering rather than conventional dislocation-mediated plasticity. Similar dissipation-free elasticity and a reproducible onset of dissipation were observed across our dataset (Supplemental Material Figs. S3–S5 and Movies S1–S3) [33].

To quantify the elastic response, we extract an effective axial Young’s modulus E for each nanodiamond from the small-strain, dissipation-free regime using the uniaxial definition:

$$E = \frac{kl}{A}, \quad (1)$$

where k is the measured stiffness, l is the initial particle height along the loading axis, and A is the effective cross-sectional area obtained from multiple chord measurements perpendicular to the loading axis. Both l and A are determined from TEM images using an effective-geometry description (see Supplemental Material Note S1.2 [33]), which also accounts for modest deviations from an ideal sphere in projection. To define A for nonideal projected shapes, we determine an effective transverse diameter D_{eff} by measuring multiple chord lengths across the particle perpendicular to the loading axis and taking their mean; the cross-sectional area is then approximated as $A = \pi(D_{\text{eff}}/2)^2$. Stiffness values were extracted from the purely elastic region, prior to the onset of plastic deformation, to avoid inaccuracies caused by incomplete contact or plasticity. Stiffness is extracted exclusively from the purely elastic window—i.e., the displacement-strain range in which the dissipation remains at the baseline level—thereby avoiding artifacts from incomplete contact at the very beginning of loading and from the onset of irreversible deformation at larger strains. Notably, Δl in $k = dF/d(\Delta l)$ is the nanoparticle shortening measured directly from TEM images; therefore, any elastic indentation of the diamond indenters does not enter the displacement axis and does not bias the extracted modulus. We note that the reported Young’s modulus should be interpreted as an effective axial

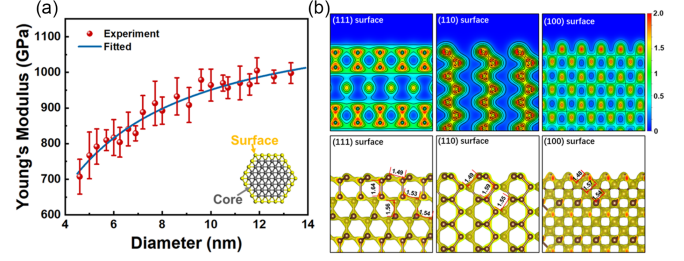


FIG. 3. Size dependence Young’s modulus of nanodiamond and first principles simulations of diamond surface. (a) Effective axial Young’s modulus of nanodiamonds as a function of particle diameter. The red dots and error bars represent the average values and standard deviations, respectively. The blue lines indicate the fitted values obtained by applying Eq. (2) to the experimental data. (b) Charge density distributions of diamond with different surface structures (isosurface at $1.5 \text{ e}/\text{\AA}^3$).

modulus under contact-constrained nanoparticle compression. For completeness, indenter compliance is naturally included in our Hertz-type consistency check via the reduced modulus E^* for a diamond–diamond contact (Supplemental Material S4.1 [33]).

A statistical analysis of ~ 100 nanodiamonds was conducted to explore the size dependence of effective axial Young’s modulus, as shown in Fig. 3(a), the error bars shown in Fig. 3(a) represent the standard deviation. A clear size-dependent reduction in effective axial Young’s modulus is observed, with E decreasing systematically as the particle diameter decreases. Nanodiamonds with diameters of ~ 12 nm exhibit $E \approx 1000$ GPa, close to the bulk value, whereas particles of ~ 4 nm show a pronounced reduction to ~ 700 GPa. At these ultrasmall sizes, the surface-to-volume ratio becomes large, so near-surface contributions are expected to increasingly influence the effective mechanical response. Importantly, re-analysis using an alternative sphere-flattening geometry commonly used in particle compression yields the same qualitative reduction in effective axial Young’s modulus trend, indicating that our main conclusion is robust against moderate deviations from ideal sphericity (Supplemental Material S2.3 [33]). In our Hertz-type consistency check we use the diamond–diamond reduced modulus E^* and convert it to the particle modulus using the known elastic constants of the diamond indenters, which explicitly accounts for the finite elastic compliance of the indenter tips at small contacts.

Although bulk diamond is elastically anisotropic, for particles whose lattice fringes enabled indexing of the apparent zone axis from preloading HRTEM FFTs (e.g., $\langle 100 \rangle$, $\langle 110 \rangle$, and $\langle 111 \rangle$), the extracted Young’s modulus does not show a systematic orientation-dependent offset within the experimental scatter.

III. DISCUSSION

To quantitatively assess this surface effect, the experimental data were analyzed using a core-shell model,

wherein a nanodiamond is considered to consist of a core region surrounded by a surface layer with a distinct Young's modulus. To parametrize the observed size dependence of the effective modulus, we adopt a simple two-region (core-surface) mixing rule as an effective description. We emphasize that the stress-strain field in a quasispherical particle compressed between flats is heterogeneous (polar contact regions versus equatorial side surfaces), so Eq. (2) should not be interpreted as a strict isostrain condition throughout the particle. The overall Young's modulus of the nanodiamond (E_{total}) can be obtained by summation of weighted Young's modulus of core (E_{core}) and surface (E_{surface}) as [18]:

$$E_{\text{total}} = E_{\text{surface}} \frac{A_{\text{surface}}}{A_{\text{total}}} + E_{\text{core}} \frac{A_{\text{core}}}{A_{\text{total}}} \quad (2)$$

where A_{core} and A_{surface} are the cross-sectional areas of the core and surface region, respectively. In this core-shell model, the surface region is defined as an outer shell of thickness t_{shell} . For a nanoparticle with effective diameter D_{eff} , the core cross-sectional area is $A_{\text{core}} = \pi(D_{\text{eff}} - 2t_{\text{shell}})^2/4$, effective diameter D_{eff} is obtained by averaging multiple chord measurements across the segmented contour. This concept has been successfully applied to other covalent or ionic-covalent nanomaterials, including ZnO and GaN nanowires, Si and SiC nanostructures, and metallic nanocontacts, where surface elasticity plays a dominant role in size-dependent mechanical behavior. The stress-strain field in a quasispherical nanodiamond compressed between two flat platens is inherently heterogeneous. The polar contact regions tend toward an isostresslike response due to traction continuity across the contact, whereas the equatorial side regions are closer to an isostrainlike response. Therefore, Eq. (2) should not be interpreted as implying a uniform strain state inside the particle or as a strict isostrain (Voigt) description of the internal field. Instead, it is introduced as a geometry-averaged and physically interpretable parametrization of an effective Young's modulus in terms of a bulklike core and a mechanically softened near-surface region.

By fitting this model to the experimental data in Fig. 3(b) using the Levenberg-Marquardt method [39], with a single (size independent) t_{shell} for all particles, we obtain $E_{\text{core}} = 1185.8 \pm 41.6$ GPa, $E_{\text{surface}} = 341.4 \pm 557.7$ GPa, and $t_{\text{shell}} = 0.75 \pm 0.63$ nm (1σ , from the fit covariance matrix). The obtained Young's modulus of the core closely matches the known bulk value for diamond (~ 1140 GPa [14]), while the surface Young's modulus is much smaller than that of the core, indicating pronounced surface compliance. Because E_{surface} and t_{shell} are strongly coupled, the absolute value of E_{surface} is sensitive to the assumed t_{shell} ; we quantify this by refitting the data with fixed t_{shell} in a physically reasonable range (0.6–1.0 nm), which

leaves the fit quality and E_{core} nearly unchanged while E_{surface} varies along the correlated direction. Full uncertainties, parameter correlations, and sensitivity or cross-validation analyses are provided in the Supplemental Material [33]. This suggests that the interatomic potential at the surface has a shallower slope compared to the core, which may be a consequence of the lower coordination number of surface atoms.

To further elucidate the atomic-scale origins of this behavior, density functional theory (DFT) calculations were carried out to investigate the atomic structures of the diamond (111), (110), and (100) surfaces, as shown in Fig. 3(b). The results reveal that the outermost surface layers exhibit the shortest C–C bond lengths, approximately 1.49 Å, while bonds in the core are close to the bulk value of about 1.55 Å. Notably, the bonds connecting the surface and subsurface layers are longer than those in the core, measuring 1.64, 1.59, and 1.57 Å for the (111), (110), and (100) surfaces, respectively. Importantly, this bond-length hierarchy is consistent with our molecular dynamics (MD) statistics obtained using the same nearest-neighbor definition and region partitioning (surface, interfacial, and core): MD likewise shows shortened bonds within the surface layer, bulklike bonds in the core, and distinctly elongated surface-subsurface (interfacial) bonds, supporting a common interfacial weakening picture across both DFT and MD analyses. These results suggest that although the bonding within the surface atomic layers appears stronger due to shorter bond lengths and higher charge density, the bonding between surface and core atoms is significantly weakened, leading to an overall lower elastic stiffness of the surface region as a structural unit. We further examined H- and O-terminated diamond surfaces by DFT and found that the near-surface structural or electronic contrast (layer-resolved C–C bond-length deviations and interfacial charge redistribution) remains pronounced for H termination but is substantially reduced for O termination; details are provided in the Supplemental Material (Figs. S11, S12).

Complementary charge density distribution analyses further corroborate these structural trends. As shown in Fig. 3(b) and Fig. S10 [33], significant charge redistribution is evident across the (111), (110), and (100) surfaces. The charge density is notably higher within the surface layers, whereas the core region exhibits a lower charge density. More importantly, a marked reduction in charge density is observed at the interface between the surface and core, further confirming the presence of weakened bonding interactions in this region. Together, these findings demonstrate that the observed lower elastic stiffness behavior of nanodiamonds does not arise from the intrinsic properties of the surface atomic layers, which actually display higher stiffness, but rather from the weakened bonding at the surface-core interface. This interfacial bonding weakening plays a decisive role in controlling the elastic properties of nanodiamonds at the nanoscale.

Molecular dynamics (MD) simulations were performed to examine their elastic response. Detailed simulation parameters and procedures are provided in Supplemental Material [33]. The simulated Young's modulus is in good agreement with our experimental one (see Fig. S13 in Supplemental Material [33]). The potential energy of surface atoms, core atoms, and the overall average for all atoms was calculated as a function of applied strain, as shown in Supplemental Material of Fig. S14 [33]. The results indicate that the surface atoms possess higher potential energy than the core atoms, while the overall average lies between these two values. The higher potential energy reflects increased stored strain energy and local bond distortion relative to the relaxed reference compared to the core, consistent with our experimental observations. Additionally, the simulations show that the elastic energy density at the surface varies significantly with particle size, whereas the elastic energy density within the core remains largely constant regardless of nanodiamond diameter (Fig. S14 [33]).

Notably, the curvature of the potential energy versus strain curves reflects the local stiffness of each region [40]. By fitting these curves with polynomial functions, we extracted the stiffness values for the surface, core, and the entire nanodiamond, allowing us to calculate the corresponding Young's modulus for each region. The resulting Young's modulus values demonstrate a clear size-dependent trend: the overall Young's modulus increases with increasing particle size. Specifically, the Young's modulus of the core is approximately 1050 GPa, while that of the surface is about 400 GPa, both in good agreement with our experimental measurements, as shown in Fig. 4(a) and Fig. S15 [33]. Interestingly, when the diameter decreases below 2 nm, the core Young's modulus exhibits a slight increase, while the surface Young's modulus decreases marginally. This behavior further confirms that surface effects play a dominant role in governing the mechanical response of smaller nanodiamonds, primarily due to changes in the atomic coordination environment at the surface.

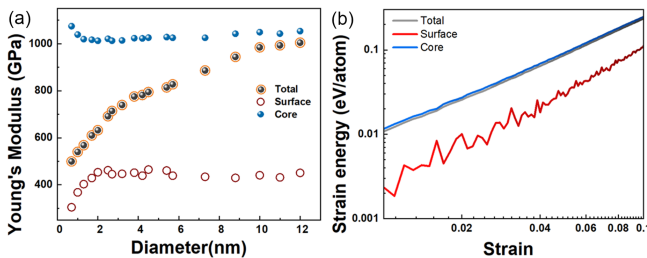


FIG. 4. Simulated Young's modulus and strain energy of the nanodiamond. (a) Simulated Young's modulus of the nanodiamond as a function of diameter, the blue, red, and gray dot indicate the Young's modulus of the core, surface, and overall nanodiamond, respectively. (b) Strain energy of the core (blue), surface (red), and overall nanodiamond (gray) as a function of applied strain.

In ultrasmall nanodiamonds, a relatively large fraction of surface atoms possesses coordination numbers of 2 or 3, in contrast to the coordination number of 4 in core atoms. As a result, the overall mechanical behavior of small nanodiamonds is predominantly dictated by these mechanically lower elastic stiffness, under-coordinated surface atoms, whereas in larger nanodiamonds, the stiffer core atoms increasingly control the elastic response.

To further elucidate the surface effect, we examined the variation of strain energy density for the surface, core, and the overall nanodiamond as a function of deformation, as presented in Fig. 4(b). The strain energy density for each region was obtained by partitioning the total strain energy into contributions from surface and core atoms and normalizing by the number of atoms within each respective region. The results indicate that the strain energy density in the core consistently exceeds that at the surface, reflecting a stiffer elastic response in the core and a comparatively reduced elastic modulus of the surface region. These findings confirm that as the particle size decreases, the effective mechanical behavior of nanodiamonds becomes progressively dominated by surface atoms. This significant reduction in elastic modulus in the near-surface region effect thus represents the primary mechanism responsible for the size-dependent elastic properties observed in brittle nanodiamonds.

The strain evolution of individual bonds under applied deformation was analyzed to directly visualize this interfacial effect at the bond level. Bond-level strain analyses are performed with an explicit orientation filter relative to the loading axis (Supplemental Material Fig. S10) [33]. The strain in surface-core connecting bonds rises more rapidly than that in either core bonds or surface bonds as total strain increases. Notably, these connecting bonds exhibit both a higher initial strain sensitivity and a larger strain accumulation under loading. In contrast, surface bonds maintain lowest strain levels throughout the entire deformation range, while core bonds display a moderate response with relatively stable behavior within the initial elastic regime. This bond-resolved strain distribution highlights the mechanical weakening at the surface-core interface, where strain localization initiates, consistent with the atomic-scale bond length and charge density analyses from DFT and the energy dissipation trends observed in MD simulations. Such strain localization facilitates local bond rearrangements and atomic sliding at the interface, forming a preferential site for plasticlike dissipation.

To rationalize these phenomena within a fracture mechanics framework, we considered the classic Griffith criterion [41], which states that crack propagation occurs when the strain energy release rate (G) exceeds twice the surface energy ($2\gamma_s$). In bulk or larger nanodiamonds, this condition is readily satisfied, leading to brittle failure. At the 4–13 nm scale studied here, however, the classical continuum notion of a sharp “crack tip” with a stress singularity is not strictly applicable; in this nanoscale

context, we use crack tip only in a crack-tip-like atomistic sense to denote the incipient interfacial decohesion-localization front where stress or strain concentrates and bond rearrangement initiates. In nanodiamonds, the presence of a weakly bonded surface-core interface promotes significant plasticlike atomic rearrangements, including surface atom sliding, bond-length adjustments, and localized structural relaxations, thereby dissipating energy and impeding cleavage-like crack advance. This aligns with the Orowan modification of the Griffith criterion [$G \geq 2(\gamma_s + \gamma_p)$] [42], which incorporates an additional term, γ_p , representing the energy dissipated through plastic deformation. Our experimental observations of plastic deformation and energy dissipation beyond the elastic limit provide direct evidence for the formation of an interfacial plastic dissipation zone that inhibits crack propagation. Taken together, these fracture mechanics frameworks consistently suggest that atomic-scale interfacial dissipation mechanisms play a critical role in governing the enhanced elastic deformation and delaying brittle fracture in nanodiamonds, thereby enabling their exceptional elasticity at the nanoscale.

Although the present measurements and simulations were performed at room temperature, the size-dependent reduction in Young's modulus is expected to remain qualitatively robust under moderate temperature variations, because it is governed primarily by the structural-bonding contrast at the surface-core interface; temperature is instead expected to shift the absolute modulus through anharmonic lattice softening, with possible deviations only when elevated temperatures induce surface reconstruction or diffusion.

IV. CONCLUSIONS

In summary, we have systematically investigated the size-dependent elastic properties of nanodiamonds through *in situ* TEM technique along with DFT and MD simulations. Our results reveal that the elastic behavior of nanodiamonds is strongly governed by surface effects, particularly in smaller particles, where a high fraction of low-coordination surface atoms induces pronounced reduced elastic modulus of the near-surface region. The effective axial Young's modulus of the nanodiamond core remains relatively constant, whereas the modulus of the surface layer decreases with decreasing particle size, leading to an overall size-dependent elastic response. Notably, this reduced elastic modulus of the near-surface region originates not from the intrinsic stiffness of the surface atomic layers—which actually exhibit stronger bonding—but from the weakened bonding at the interface between the surface and the core. This study highlights the crucial role of atomic coordination environments in governing the mechanical response at the nanoscale and provides valuable insights into the fundamental mechanics of brittle nanomaterials. These findings not only provide a fundamental understanding of the size-dependent elasticity

in nanodiamond, but also offer valuable guidance for the design of nanoresonators with tunable frequency response and for thermal transport devices where interface-modulated phonon scattering is crucial. More broadly, our results suggest that, in ultrastiff covalent nanocrystals, elasticity can be governed by a mechanically distinct surface-core interfacial zone rather than the outermost surface alone, offering a tunable knob via surface state or termination for stiffness-dissipation engineering. These results suggest practical knobs for nanoscale devices—nanomechanical resonators, phononic elements, and diamond-based quantum sensors—where size or surface-controlled stiffness can tune resonance or impedance while operating below the dissipation onset helps maximize Q and suppress loss.

V. METHODS

A. Sample preparation and structure characterization

The experiment in this study was conducted using a custom-designed TEM holder [Fig. 1(a)], equipped with a self-sensing AFM probe based on LER. For mechanical measurements, nanodiamonds were clamped between two diamond indenters: one affixed to a 10 μm diameter tungsten tip glued to the edge of the LER prong (3EXW-1073, STATEK), and the other mounted on a 100 μm diameter tungsten tip fixed to the holder frame. The nanodiamonds, synthesized via a detonation method and with diameters below 10 nm, were cleaned in aqua regia for at least 24 h to remove surface sp^2 carbon, and subsequently dispersed onto the surface of one of the diamond indenters. To evaluate the mechanical response of the nanoparticles during deformation, the LER prong was driven to oscillate at its resonance frequency (f_0 , ~ 1 MHz) with an amplitude of approximately 15 pm by applying a sinusoidal excitation voltage using a phase-locked loop. The actuation voltage was expressed as $V^* = V e^{i\omega t}$ (V is the amplitude of the applied voltage, ω is frequency, t is the time and i is the imaginary unit). As a result, the LER oscillated with a displacement of $a^* = a e^{(i\omega t + \varphi)}$, where a is the oscillate amplitude and φ is the phase shift between the driving force and the response. The mechanical behavior of the nanodiamonds was characterized by the complex stiffness $k^* = (F^*/a^*) = k e^{-i\varphi}$, where k' (real part) and k'' (imaginary part) represent the conservative (elastic) and dissipative (plastic) responses of the material, respectively [32,44–46].

$$k_{\text{sample}} = 2k_{\text{LER}} \frac{\Delta f}{f_0}. \quad (3)$$

The dissipative energy associated with the LER reflects the energy loss during the deformation of the sample and is directly related to the imaginary component of the stiffness. This dissipation is indicative of plastic deformation in the

sample and can be quantified based on the LER excitation voltage $[V(A)]$:

$$E_{\text{diss}} = \frac{\pi k_{\text{LER}} A^2}{Q} \left(\frac{V(A)}{V_0(A)} - 1 \right), \quad (4)$$

where the Q is the quality factor of LER, A is the oscillation amplitude, and $V_0(A)$ is the excitation voltage required to maintain that amplitude in the absence of a connected sample. During loading, the resonance frequency f_0 and quality factor Q are continuously tracked by a phase-locked loop (PLL), which keeps the LER driven at resonance; slow drifts are therefore compensated in real time, and we analyze baseline-referenced increments (Δf) relative to the pre-contact state. Equation (3) follows the standard small-perturbation (linear) FM formulation and is valid when the contact-induced stiffness satisfies to the regime where $\Delta f/f_0$ remains small (typically $\leq 5\%$, corresponding to $k_{\text{ts}}/k_{\text{LER}} \leq 5\%$). The free resonance parameters (f_0 , Q , and k_{LER}) are calibrated *in situ* in the TEM vacuum using the thermal-noise method [18,27–29].

Owing to the high stiffness of LER, the overall mechanical response is dominated by the specimen rather than by the compliance of the force sensor itself. As a result, parasitic deformation of the sensor is strongly suppressed, reducing measurement artifacts and avoiding the apparent reduction in stiffness that can arise when more compliant silicon cantilevers are used to probe materials with extremely high elastic moduli. By operating the LER in a frequency-modulation mode, the effective stiffness of the tip-sample contact can be measured directly from the resonance frequency shift.

Scanning transmission electron microscopy (STEM) measurements were conducted using a spherical-aberration-corrected microscope (JEM-ARM300F2) operated at an accelerating voltage of 300 kV. Annular bright-field (ABF) images of the diamond NPs (Fig. 1) confirm their excellent crystallinity.

In-situ TEM observations were conducted using an ultrahigh vacuum TEM (UHV-TEM, JEM-2000VF, 200 kV, 10^{-7} Pa) to minimize contamination and gas adsorption on the sample. Precise positioning of the indenter on the LER was achieved using a tube piezo actuator for fine adjustment and an ultrasonic linear motor for coarse motion. Electrical excitation and signal detection of the LER were accomplished by connecting its two electrodes via coaxial cables. The resonant frequency and oscillation amplitude of the LER were controlled and monitored using an oscillation controller (Nanonis OC4, SPECS) operating at a sampling rate of 2.4 kHz. Prior to the experiments, the samples were baked at approximately 100 °C for at least 24 h to ensure surface cleanliness. All observations were performed at room temperature (~ 300 K), and TEM images were recorded at 0.2 sec intervals using a charge-coupled device (CCD) camera.

B. Density functional theory simulation

First-principles calculations based on DFT were carried out using the CASTEP code to investigate the electronic properties of diamond surfaces. Slab models of the (111), (110), and (100) diamond surfaces were constructed, and their optimized atomic structures are shown in Fig. S10 [33]. The Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional within the generalized gradient approximation (GGA) was employed in conjunction with ultrasoft pseudopotentials. A plane-wave cutoff energy of 653 eV was used, and the Brillouin zone was sampled using a Monkhorst-Pack grid with a spacing of $0.04 \text{ \AA}^{-1}$. Convergence criteria for geometry optimization were set as follows: a maximum interatomic force of $0.03 \text{ eV/\AA}$, a maximum atomic displacement of $0.001 \text{ \AA}$, total energy convergence of $1 \times 10^{-5} \text{ eV}$, and maximum internal stress of 0.05 GPa . These criteria ensured fully relaxed and energetically stable surface configurations.

C. Molecular dynamics simulation

The deformation behavior of spherical diamond NPs was investigated using classical MD simulations, performed with the LAMMPS package [47]. The nanodiamonds were generated from pristine bulk single crystals, with diameters ranging from sub-1 nm to 12 nm. Shrink-wrapped boundary conditions were applied in all three spatial directions (x, y, z) during the simulations. Interatomic interactions were modeled using the Tersoff potential [48], which is widely recognized for its ability to capture dislocation activities and bond rearrangements in covalently bonded systems. The temperature was maintained at 300 K using velocity rescaling, and the time step was set to 1 fs. Atomic motion followed classical Newtonian dynamics and was integrated using the velocity-Verlet algorithm. The simulation protocol included the following three steps: (i) The initial atomic configuration was relaxed using the conjugate gradient method to eliminate unfavorable atomic overlaps and ensure a physically reasonable structure. (ii) The structure was equilibrated at 300 K under the NVT ensemble for 100 ps, with a temperature damping constant of 0.1 ps, allowing the system to reach thermal stability. (iii) The equilibrated NP was positioned between a rigid flat surface and a flat hard indenter. Compression was applied by driving the indenter downward at a strain rate of 10^7 s^{-1} , a value commonly used in indentation simulations. To examine whether the high strain rate could influence the apparent Young's modulus, we performed additional simulations at a lower strain rate of 10^6 S^{-1} . Within numerical uncertainty, the extracted elastic modulus and its size dependence were essentially identical to those obtained at the higher strain rate. This indicates that the modulus reported here reflects the quasi-elastic response of the system rather than rate-dependent effects. During this process, atomic trajectories and stress evolution were

recorded to track structural changes and quantify deformation responses. We further verified, using identical surface, interface, or core definitions and nearest-neighbor criteria, that the MD bond-length statistics are consistent with the DFT results, providing an internal consistency check before combining DFT (bonding or termination) and MD (size dependence) in our interpretation.

In the MD analysis, “surface”, “interface”, and “core” atoms are identified using physically motivated local descriptors rather than an *ad hoc* label, combining a depth-from-surface criterion (within a few atomic layers) with local bonding-order metrics (coordination and tetrahedral order). Varying the classification thresholds within a reasonable range does not change the main conclusions, and an independent carbon potential (LCBOP) reproduces the same qualitative size-dependent softening trend.

ACKNOWLEDGMENTS

This work was financially supported by the National Natural Science Foundation of China (Grants No. 12304050, No. 52572052, No. 12474036, No. 12274371, No. 12504039, No. U21A2070), Cross-Disciplinary Innovative Research Group Project of Henan Province (Grant No. 232300421004), Natural Science Foundation of Henan Province (Grants No. 242300421669 and No. 252300421213), The Science and Technology Innovation Leading Talent Program of Henan Province (Grant No. 254000510060) China Postdoctoral Science Foundation (Grants No. 2023M743227, No. 2025T180932), International Science and Technology Cooperation in Henan Province (No. 261111521100).

C. S. and S. C. conceived the idea, designed the experiments, and supervised the project; J. Z. performed the *in situ* TEM experiments; J. Z., C. L., X. L., and Y. O. performed the TEM characterization; J. Z. and D. W. performed the computational studies. C. S., S. C., J. Z., K. Z., and H. J. analyzed the data and wrote the manuscript. All authors contributed to data interpretation and discussed the results.

Authors declare that they have no competing interests.

DATA AVAILABILITY

The data that support the findings of this article are openly available [49].

-
- [1] T. M. Babinec, B. J. M. Hausmann, M. Khan, Y. Zhang, J. R. Maze, P. R. Hemmer, and M. Lončar, *A diamond nanowire single-photon source*, *Nat. Nanotechnol.* **5**, 195 (2010).
 - [2] B. S. Miller, L. Bezing, H. D. Gliddon, D. Huang, G. Dold, E. R. Gray, J. Heaney, P. J. Dobson, E. Nastouli,

- J. J. L. Morton *et al.*, *Spin-enhanced nanodiamond biosensing for ultrasensitive diagnostics*, *Nature (London)* **587**, 588 (2020).
- [3] S. Hsieh, P. Bhattacharyya, C. Zu, T. Mittiga, T. J. Smart, F. Machado, B. Kobrin, T. O. Höhn, N. Z. Rui, M. Kamrani, S. Chatterjee, S. Choi, M. Zaletel, V. V. Struzhkin *et al.*, *Imaging stress and magnetism at high pressures using a nanoscale quantum sensor*, *Science* **366**, 1349 (2019).
- [4] M. Fujiwara, S. Sun, A. Dohms, Y. Nishimura, K. Suto, Y. Takezawa, K. Oshimi, L. Zhao, N. Sadzak, Y. Umehara, Y. Teki, N. Komatsu, O. Benson *et al.*, *Real-time nanodiamond thermometry probing in vivo thermogenic responses*, *Sci. Adv.* **6**, eaba9636 (2020).
- [5] E. A. Ekimov, V. A. Sidorov, E. D. Bauer, N. N. Mel'nik, N. J. Curro, J. D. Thompson, and S. M. Stishov, *Superconductivity in diamond*, *Nature (London)* **428**, 542 (2004).
- [6] K. Qiu, J. Hou, S. Chen, X. Li, Y. Yue, B. Xu, Q. Hu, L. Liu, Z. Yang, A. Nie *et al.*, *Self-healing of fractured diamond*, *Nat. Mater.* **22**, 1317 (2023).
- [7] C. Dang, J.-P. Chou, B. Dai, C.-T. Chou, Y. Yang, R. Fan, W. Lin, F. Meng, A. Hu, J. Zhu *et al.*, *Achieving large uniform tensile elasticity in microfabricated diamond*, *Science* **371**, 76 (2021).
- [8] A. Banerjee, D. Bernoulli, H. Zhang, M.-F. Yuen, J. Liu, J. Dong, F. Ding, J. Lu, M. Dao, W. Zhang *et al.*, *Ultralarge elastic deformation of nanoscale diamond*, *Science* **360**, 300 (2018).
- [9] A. Nie, Y. Bu, P. Li, Y. Zhang, T. Jin, J. Liu, Z. Su, Y. Wang, J. He, Z. Liu *et al.*, *Approaching diamond's theoretical elasticity and strength limits*, *Nat. Commun.* **10**, 5533 (2019).
- [10] C. Liu, K. Yang, J. Zhang, S. Cheng, and Chongxin Shan, *In-situ transmission electron microscopy shedding light on the mechanical properties of nanoscale materials*, *Microstructures* **4**, 2024055 (2024).
- [11] A. Nie, Y. Bu, J. Huang, Y. Shao, Y. Zhang, W. Hu, J. Liu, Y. Wang, B. Xu, Z. Liu *et al.*, *Direct observation of room-temperature dislocation plasticity in diamond*, *Matter Radiat. Extremes* **2**, 1222 (2020).
- [12] Y. Wang, L. Wang, H. J. Joyce, Q. Gao, X. Liao, Y. Mai, H. H. Tan, J. Zou, S. P. Ringer, H. Gao *et al.*, *Super deformability and young's modulus of gaas nanowires*, *Adv. Mater.* **23**, 1356 (2011).
- [13] G. López-Polín, C. Gómez-Navarro, V. Parente, F. Guinea, M. I. Katsnelson, F. Pérez-Murano, and J. Gómez-Herrero, *Increasing the elastic modulus of graphene by controlled defect creation*, *Nat. Phys.* **11**, 26 (2015).
- [14] C. A. Klein and G. F. Cardinale, *Young's modulus and Poisson's ratio of CVD diamond*, *Diam. Relat. Mater.* **2**, 918 (1993).
- [15] R. Pastorelli, A. C. Ferrari, M. G. Beghi, C. E. Bottani, and J. Robertson, *Elastic constants of ultrathin diamond-like carbon films*, *Diam. Relat. Mater.* **9**, 825 (2000).
- [16] J. Diao, K. Gall, and M. L. Dunn, *Surface-stress-induced phase transformation in metal nanowires*, *Nat. Mater.* **2**, 656 (2003).
- [17] J. B. Hannon, S. Kodambaka, F. M. Ross, and R. M. Tromp, *The influence of the surface migration of gold on the growth of silicon nanowires*, *Nature (London)* **440**, 69 (2006).

- [18] J. Zhang, M. Tomitori, T. Arai, and Y. Oshima, *Surface effect on young's modulus of sub-two-nanometer gold [111] nanocontacts*, *Phys. Rev. Lett.* **128**, 146101 (2022).
- [19] Q. Yu, Z.-W. Shan, J. Li, X. Huang, L. Xiao, J. Sun, and E. Ma, *Strong crystal size effect on deformation twinning*, *Nature (London)* **463**, 335 (2010).
- [20] Y. Oshima, A. Onga, and K. Takayanagi, *Helical gold nanotube synthesized at 150 K*, *Phys. Rev. Lett.* **91**, 205503 (2003).
- [21] Y. Kondo and K. Takayanagi, *Synthesis and characterization of helical multi-shell gold nanowires*, *Science* **289**, 606 (2000).
- [22] L. G. Zhou and H. Huang, *Are surfaces elastically softer or stiffer?*, *Appl. Phys. Lett.* **84**, 1940 (2004).
- [23] R. E. Miller and V. B. Shenoy, *Size-dependent elastic properties of nanosized structural elements*, *Nanotechnology* **11**, 139 (2000).
- [24] M. D. Uchic, *Sample dimensions influence strength and crystal plasticity*, *Science* **305**, 986 (2004).
- [25] X. Jiang, J. Zhao, and X. Jiang, *Mechanical and electronic properties of diamond nanowires under tensile strain from first principles*, *Nanotechnology* **22**, 405705 (2011).
- [26] O. A. Williams, A. Kriele, J. Hees, M. Wolfer, W. Müller-Seibert, and C. E. Nebel, *High Young's modulus in ultra thin nanocrystalline diamond*, *Chem. Phys. Lett.* **495**, 84 (2010).
- [27] J. Zhang, K. Ishizuka, M. Tomitori, T. Arai, and Y. Oshima, *Atomic scale mechanics explored by in situ transmission electron microscopy with a quartz length-extension resonator as a force sensor*, *Nanotechnology* **31**, 205706 (2020).
- [28] J. Zhang, K. Ishizuka, M. Tomitori, T. Arai, K. Hongo, R. Maezono, E. Tosatti, and Y. Oshima, *Peculiar atomic bond nature in platinum monatomic chains*, *Nano Lett.* **21**, 3922 (2021).
- [29] C. Liu, K. Hongo, R. Maezono, J. Zhang, and Y. Oshima, *Stiffer bonding of armchair edge in single-layer molybdenum disulfide nanoribbons*, *Adv. Sci.* **10**, 2303477 (2023).
- [30] L. Canale, J. Comtet, A. Niguès, C. Cohen, C. Clanet, A. Siria, and L. Bocquet, *Nanorheology of interfacial water during ice gliding*, *Phys. Rev. X* **9**, 041025 (2019).
- [31] J. Comtet, A. Lainé, A. Niguès, L. Bocquet, and A. Siria, *Atomic rheology of gold nanojunctions*, *Nature (London)* **569**, 393 (2019).
- [32] J. Hong, Y. Tian, T. Liang, X. Liu, Y. Song, D. Guan, Z. Yan, J. Guo, B. Tang, D. Cao *et al.*, *Imaging surface structure and premelting of ice Ih with atomic resolution*, *Nature (London)* **630**, 375 (2024).
- [33] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/b3h5-34wt> for details of structural characterization, *in situ* TEM experiment, density functional theory, and molecular dynamics simulation, which includes Refs. [34–37].
- [34] D. Stauffer, A. Beaber, A. Wagner, O. Ugurlu, J. Nowak, K. A. Mkhoyan, S. Girshick, and W. Gerberich, *Strain-hardening in submicron silicon pillars and spheres*, *Acta Mater.* **60**, 2471 (2012).
- [35] F. Xu, Q. Qin, A. Mishra, Y. Gu, and Y. Zhu, *Mechanical properties of ZnO nanowires under different loading modes*, *Nano Res.* **3**, 271 (2010).
- [36] J. Wang, J. Schwenger, A. Ströbel, P. Feldner, P. Herre, S. Romeis, W. Peukert, B. Merle, and N. Vogel, *Mechanics of colloidal supraparticles under compression*, *Adv. Sci.* **7**, eabj0954 (2021).
- [37] A. Sharma, N. Gazit, L. Klinger, and E. Rabkin, *Pseudoelectricity of metal nanoparticles is caused by their ultrahigh strength*, *Adv. Funct. Mater.* **30**, 1807554 (2020).
- [38] J. M. Wheeler, R. Raghavan, J. Wehrs, Y. Zhang, R. Erni, and J. Michler, *Approaching the limits of strength: Measuring the uniaxial compressive strength of diamond at small scales*, *Nano Lett.* **16**, 812 (2016).
- [39] C. Kanzow, N. Yamashita, and M. Fukushima, *Levenberg–Marquardt methods with strong local convergence properties for solving nonlinear equations with convex constraints*, *J. Comput. Appl. Math.* **172**, 375 (2004).
- [40] J. H. Rose, J. Ferrante, and J. R. Smith, *Universal binding energy curves for metals and bimetallic interfaces*, *Phys. Rev. Lett.* **47**, 675 (1981).
- [41] A. A. Griffith and G. I. Taylor, *The phenomenon of rupture and flow in solids*, *Phil. Trans. R. Soc. A* **221**, 163 (1921).
- [42] E. Orowan, *Fracture and strength of solids*, *Rep. Prog. Phys.* **12**, 185 (1949).
- [43] G. R. Irwin, *Analysis of stresses and strains near the end of a crack traversing a plate*, *J. Appl. Mech.* **24**, 361 (1957).
- [44] F. J. Giessibl, *Forces and frequency shifts in atomic-resolution dynamic-force microscopy*, *Phys. Rev. B* **56**, 16010 (1997).
- [45] D. Wu, Z. Zhao, B. Lin, Y. Song, J. Qi, J. Jiang, Z. Yuan, B. Cheng, M. Zhao, Y. Tian *et al.*, *Probing structural superlubricity of two-dimensional water transport with atomic resolution*, *Science* **384**, 1254 (2024).
- [46] J. Comtet, A. Lainé, A. Niguès, L. Bocquet, and A. Siria, *Atomic rheology of gold nanojunctions*, *Nature (London)* **569**, 393 (2019).
- [47] P. Steve, *Fast parallel algorithms for short-range molecular dynamics*, *J. Comput. Phys.* **117**, 1 (1995).
- [48] J. Tersoff, *New empirical approach for the structure and energy of covalent systems*, *Phys. Rev. B* **37**, 6991 (1988).
- [49] J. Zhang, C. Liu, X. Li, D. Wang, K. Zhao, H. Ji, Y. Oshima, S. Cheng, and C. Shan, *Supporting data for “Subsurface driven size-dependent elasticity in nanodiamond”*, [10.6084/m9.figshare.31810438](https://figshare.com/10.6084/m9.figshare.31810438).