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# Soft-Mode Scenarios of Shear Localization: Atomic-Level Landscapes

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Using an elementary case study of stress-induced structural instability in a crystal we discuss how collective response to large-strain deformation at the atomic level can give insights into the mechanistic nature of shear localization. Stability criteria and reaction pathway sampling are used to probe saddle-point configurations, both local spatial coordinates and activation energy barriers, to optimally extract the information available from molecular dynamics simulations.

**KEY WORDS:** shear instability in solids, stress-induced structural transitions, shear localization, dislocation slip and deformation twin, atomic-level insights, atomistic simulations, scenarios of localization phenomena

## 1. INTRODUCTION

We begin with a few words to motivate this Commentary, written on the occasion of seventieth birthday celebration of Pierre Hohenberg and Jim Langer in appreciation of their seminal contributions to the theory of condensed matter. The problem we propose to examine is the atomic-level understanding of how crystals undergo large-strain deformation to reach a point of instability. This is surely a phenomenon that occurs in all physical systems; nonetheless there are still issues not well understood. The ones we consider here have to do with probing the highly non-equilibrium states in a many-body system through dynamical simulations, and finding one's way in and out of a saddle-point. We are interested in the intrinsic or ideal behavior of the system, which means the crystal has no defects and the deformation is homogeneous. These are the conditions generally accessible only by simulation.

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In the process of applying a uniform stress to a perfect crystal to drive it over a saddle point into a final state, three basic questions always come up in the analysis. How can one predict the critical value of the forcing field? How can one search for the atomic configurations and energy of the saddle point? How can one understand the transition to the final state if it is not prescribed *a priori*? Even though a perfect crystal is an elementary system, the conceptual implications of these questions are no less relevant than the complex issues confronting current developments in the theory of condensed matter.

## 2. INSTABILITY IN NANO-INDENTATION (AN EXAMPLE)

We proceed with a specific case study—the observation of dislocation nucleation in nano-indentation experiments. A single crystal, subjected to a local external stress through the action of the indenter, deforms in a manner shown in Fig. 1.[1] The variation of the compressive stress with depth of indentation, typically seen in such measurements, shows a continuous increase of depth with load as expected in elastic deformation, with intermittent *discontinuous* jumps which suggest the loss of structural stability in a local region. These have been

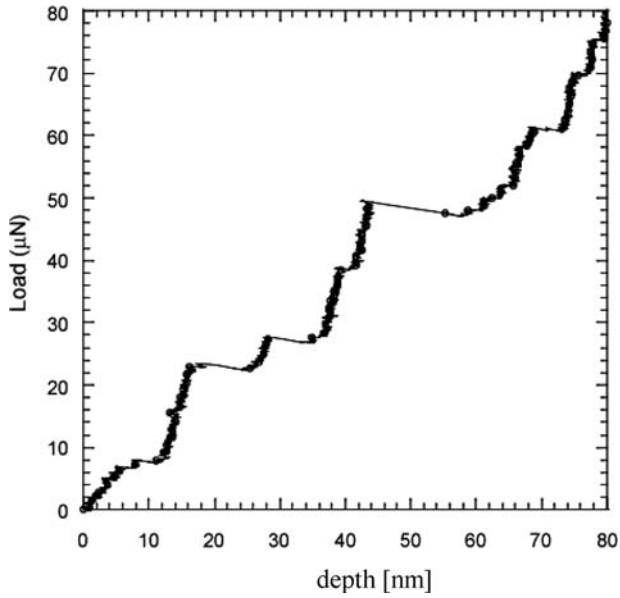


**Fig. 1.** Typical load–displacement curve in a nano-indentation measurement (load control).[1] Continuous increase of indentation depth with indenter loading shows elastic deformation interspersed with horizontal jumps. These "bursts" are interpreted as the onset of dislocation activity, each jump corresponding to a local instability somewhere in the system (not necessarily right under the indenter).

regarded as onsets of plastic deformation, in the form of dislocation nucleation and multiplication events.

To interpret Fig. 1 from a statistical mechanics perspective, we note the problem at hand is one of mechanical instability and not of phase transition, given that the final state of each burst is not prescribed *a priori*. Nevertheless, an order parameter could be useful to characterize the process and provide a means to quantify critical loading. Suppose one takes the elastic modulus as the order parameter and looks for a loading stress that makes this quantity vanish. This is essentially the basis of the Born elastic stability criterion.[2] Strictly speaking, Born considered the situation of zero applied stress, but the modulus can still vanish under another control parameter such as temperature. The proper criterion is governed by the elastic stiffness matrix B,[3,4]

$$B_{ijkl} = C_{ijkl} + \frac{1}{2}(\delta_{ik}\sigma_{jl} + \delta_{jk}\sigma_{il} + \delta_{il}\sigma_{jk} + \delta_{jl}\sigma_{ik} - 2\delta_{kl}\sigma_{ij}) \tag{1}$$

with $C_{ijkl}$ being the isothermal elastic constant tensor evaluated in the current state and $\sigma_{ij}$ the external stress. For a cubic crystal under hydrostatic stress the requirement of positivity of B leads to

$$C_{11} + 2C_{12} + P > 0, \quad C_{11} - C_{12} - 2P > 0, \quad C_{44} - P > 0 \tag{2}$$

where $C_{ij}$ are the usual elastic constants, and $P > 0 (< 0)$ denotes compression (tension). The first condition in (2) ensures stability in cohesion (finite bulk modulus), while the second and third inequalities imply positive tetragonal and rhombohedral shear moduli respectively (stability in shear). These simple criteria have been helpful in elucidating simulation results on structural phase stability.[3,5]

## 3. A LOCAL CRITERION FOR DEFECT NUCLEATION

The elastic stability criteria (2) apply to a perfect crystal under *homogeneous* deformation. For *inhomogeneous* deformation such as the case of nanoindentation, one expects local defects to be nucleated at certain sites in the system (the weak spots) when the system is driven across a saddle point. A continuum-level description of homogeneous nucleation was first explored by R. Hill[6] in the concept of discontinuity of "acceleration waves." Later J. R. Rice[7] treated shear localization in much the same spirit and derived a formal criterion characterized by a tensor **L** playing the same role as the stiffness tensor **B**. This formalism can be taken to the discrete-particle level to obtain a spatially-dependent nucleation criterion for practical implementation.[8,9] Consider a representative volume element (RVE) undergoing homogeneous deformation at finite strain to a current configuration **x**. Expanding the free energy $F$ to second order in incremental displacement

$\mathbf{u}(\mathbf{x})$, one obtains

$$\Delta F = \frac{1}{2}\int_{V(\mathbf{x})} D_{ijkl}u_{i,j}(\mathbf{x})u_{k,l}(\mathbf{x})\,\mathrm{d}V \tag{3}$$

where $D_{ijkl} = C_{ijkl} + \tau_{jl}\delta_{ik}$, $\tau_{ij}$ being the internal (Cauchy) stress, and $u_{i,j} \equiv \partial u_i(\mathbf{x})/\partial x_j$. In Eq. (3) $C$ is the elastic constant tensor and $\mathbf{u}(\mathbf{x})$ the strain at the current state of stress. By resolving the displacement as a plane wave, $u_i(x) = w_i e^{ik\cdot x}$, one arrives at the stability condition for the RVE,

$$\Lambda(\mathbf{w}, \mathbf{k}) = (C_{ijkl}w_i w_k + \tau_{jl})k_j k_l > 0 \tag{4}$$

The structure of Eq. (4) is analogous to that of the stiffness tensor $\mathbf{B}$, the presence of the stress term represents the work done by the external load.[3] Whereas $\mathbf{B}$ determines the overall crystal stability in homogeneous deformation, $\Lambda$ is in contrast a site-dependent quantity, with its sign indicating the concavity of $F$. The significance of Eq. (4) is that if a pair of $\mathbf{w}$, $\mathbf{k}$ exists such that $\Lambda$ vanishes or becomes negative, then homogeneity of the RVE cannot be maintained and a defect singularity will form internally. In other words, the inequality can be used to interrogate the elastic stability of the RVE by minimizing $\Lambda$ with respect to the polarization vector $\mathbf{w}$ and the wave vector $\mathbf{k}$. The minimum value of $\Lambda$, $\Lambda_{\min}$, acts as a measure of the *local micro-stiffness*; wherever $\Lambda_{\min}$ vanishes, an instability is predicted at that spatial position. Equation (4) is an energy-based criterion applicable to finite-strain deformation, with the minimization of $\Lambda$ being the process where the local environment is sampled from point to point. Notice that the Helmholtz form of the free energy is used rather than the Gibbs form. This is because we are applying the plane wave resolution effectively in an RVE, the region containing the weak spot, with periodic boundary condition, so no external work is involved.[5]

The usefulness of Eq. (4) has been demonstrated in analysis of MD simulation results on nano-indentation.[7,8] The first few predictions of instability according to the $\Lambda$ criterion were found to correspond closely with jumps in the simulated load-displacement curve, as shown in Fig. 2. Because the simulations were performed at increments of fixed strain (displacement control mode), discontinuities appear as vertical jumps in contrast to Fig. 1. We refer interested readers elsewhere[8–10] for further discussions of atomic-level understanding of dislocation nucleation and propagation in nano-indention.

## 4. PROBING SHEAR DEFORMATIONS – DISLOCATION SLIP VERSUS TWINNING

Slip and twinning of crystal planes are competing processes by which a crystal can plastically accommodate large shear strains. They are distinguished by the number of planes which undergo sliding, as indicated schematically in

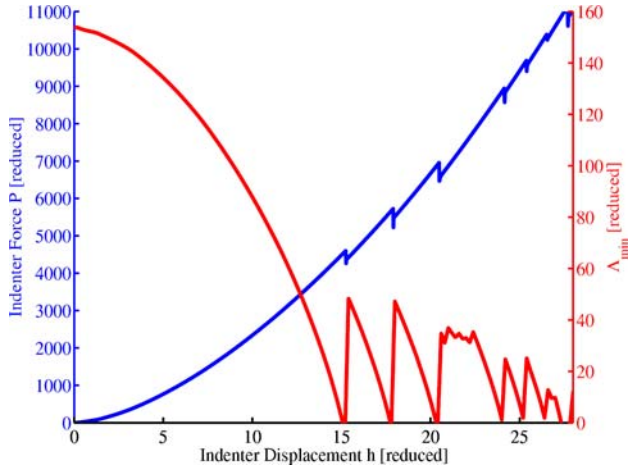


**Fig. 2.** Load-displacement response in an MD simulation of nano-indentation (load control) on a slab of single crystal of Cu (rising curve), showing several vertical jumps corresponding to the dislocation bursts of Fig. 1.[7] The decreasing curve gives the variation of $\Lambda_{min}$ with indenter depth. According to Eq.(4), each vanishing of $\Lambda_{min}$ signals a structural instability.

Fig. 3. In the lattice response to shear; slip refers to *only one* relative displacement between two adjacent layers, while for twinning a stack of *three or more layers* must undergo uniform shear. When a crystal is being sheared uniformly, all the planes initially respond elastically. This would continue until symmetry is broken, when the system spontaneously transforms into a crystal containing a defect (loss of homogeneity). In practice considerations of factors such as the crystal structure and the material in question, the planes on which deformation is taking place, the temperature and the shear rate allow one to predict on the basis of conventional wisdom whether slip or twinning is favored. In the absence of such knowledge,

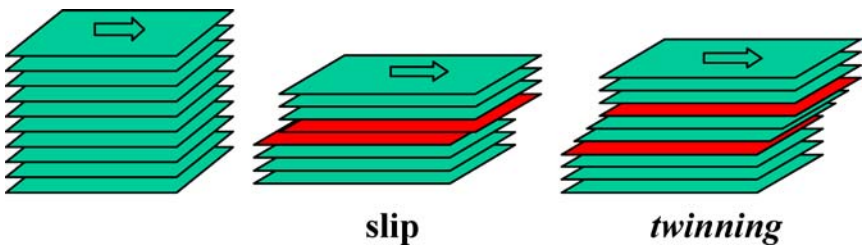


**Fig. 3.** Schematic of a stack of undeformed crystal planes (left) about to undergo shear localization. A dislocation is nucleated by a *single* relative displacement (middle), whereas twinning requires *two or more* consecutive relative displacements (right, three displacements).

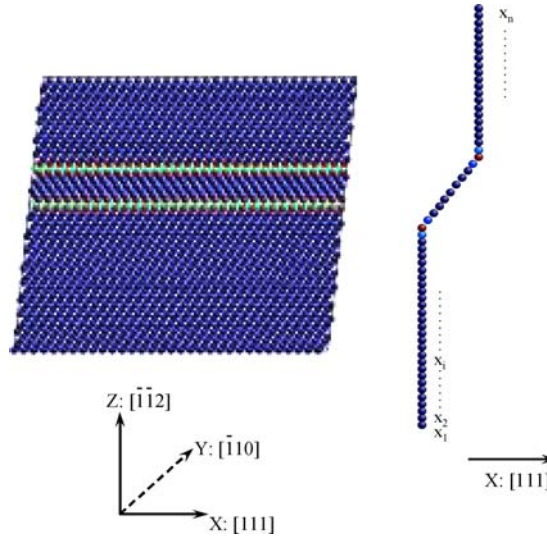


**Fig. 4.** A 3D crystal in shear along the X axis containing a twinned region of 7 planes, bounded by two twin boundaries (left). Schematic of the 1-D chain model with 9 twinned layers (in this illustration).[11,12]

one can resort to simulation for observing the atomistic details concerning system response near a saddle point.

Molecular dynamics (MD) simulations have been performed to observe the spontaneous nucleation of a deformation twin in a bcc crystal.[11,12] A simulation cell containing 500,000 atoms with periodic boundary conditions is chosen to have the the X (horizontal), Y (normal to plane of paper) and Z (vertical) axes oriented as shown in Fig. 4. Shear is applied at $3 \times 10^6$ $s^{-1}$ on the xy plane in the X (twinning) direction, extremely fast by laboratory standards but quite slow by MD standards. At 10 K we observe homogeneous nucleation of a deformation twin at a critical shear stress of 12.2 GPa (7.8% strain). Once nucleation sets in, a sharp decrease in strain energy and shear stress is observed. The full 3D configuration of the twinned crystal has too many degrees of freedom to be efficiently processed in any kind of detailed analysis. Given that the twinned region is well localized, an overwhelming majority of the particles are not relevant for the characterization of defect configuration and energy. We therefore introduce a 1D chain model to single out those coordinates essential to define the twin structure. As indicated in Fig. 4, we regard the twin as a one-dimensional chain of 'defect atoms' specified by a set of coordinates $x_i$, measured on the X-axis in the twinning direction. Each 'defect atom' i represents a plane of physical atoms, the layer being perpendicular to the chain direction, with coordinates $(x_i, y_i, z_i)$. In this model the

only degrees of freedom are the *relative displacements* in the twinning direction *between adjacent layers*, that is, $\Delta x_i = x_{i+1} - x_i$. For a twin consisting of N relative displacements of 'defect atoms', there are *N primary* degrees of freedom, $\Delta x_i$, $i = 1, \ldots, N$, specifying the defect. All the other degrees of freedom, the relative displacements in the Y and Z directions will be considered frozen and taken out of the analysis. The system energy is therefore only a function of N variables, $E = E(0, \ldots 0, \Delta x_j, \ldots, \Delta x_{j+N}, 0, \ldots 0)$, with the displaced planes starting at position j and ending at $j + N$.

Using the chain model, with the energy functional $E(\Delta x_1, \ldots, \Delta x_N)$ evaluated numerically treating all the degrees of freedom except $\Delta x_1, \ldots, \Delta x_N$ in the three-dimensional crystal as either frozen or under constrained relaxation, one has a means to examine the energetics of the twin defect for an arbitrary number of layers undergoing relative displacements. The simplest case is the 1-component chain involving a rigid translation of the upper half of the lattice relative to the lower half. The one-dimensional energy $E(0, \ldots, \Delta x_1, \ldots 0)$, allowing relaxation in the other two directions, is conventionally known as the $\gamma$-surface, a quantity commonly used to characterize lattice deformation in shear. The 2-component chain is the one of present interest, as it is able to describe either a one-layer slip or a two-layer twin. The two-dimensional energy surface is shown in Fig. 5, where a minimum is now seen around the displacements (b/3, b/3).[12] The significance is that under positive shear the present system can either twin or slip. The energy barrier for twinning is found to be 0.672 eV with the saddle point at (0.36b, 0.16b), while for slip the barrier is 0.736 eV with the saddle point at (0.5b, 0.09b). Under negative shear, only slip is allowed, at a barrier of 0.808 eV. This is the kind of atomic-level energy landscape that enables one to analyze the competition between dislocation slip and deformation twin. Another useful way to examine the energy surface is in the form of a contour plot, also shown in Fig. 5. In this one can trace out the minimum-energy path for the two deformations, using any of the reaction pathway techniques in the literature. The particular result given here was obtained by the method of nudged elastic band.[13] The path is seen to connect the initial configuration at the perfect lattice energy minimum (0,0) with the two possible final-state configurations, an energy minimum corresponding to a 2-layer twin at (b/3, b/3), and another minimum corresponding to a dislocation slip at (b, 0). The two paths bifurcate at (0.29b, 0.03b) before either of the saddle points is encountered. The system can either twin or slip after the bifurcation point; however, since the twinning path has a lower energy barrier than the slip path, 0.672eV to 0.736eV, twinning is expected to be favored.

## 5. STRAIN LOCALIZATION

In our MD simulation the process which revealed the formation of a twin involved the application of a uniform shear strain to a perfect crystal in incremental

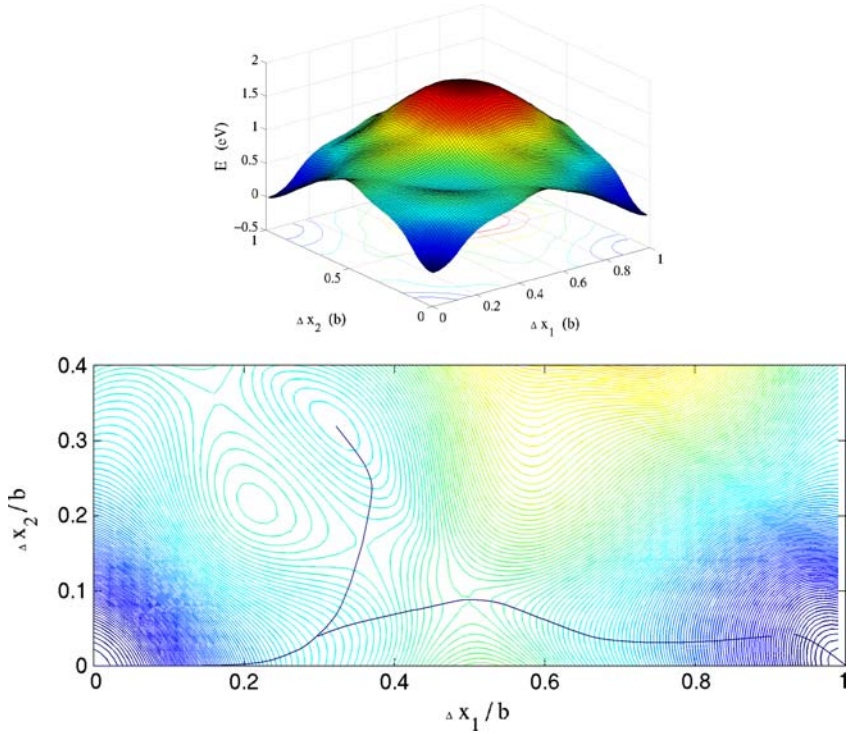


**Fig. 5.** Strain energy surface (upper) and energy contour plot (lower) for the $(\bar{1}\bar{1}2)[111]$ deformation, with Y and Z relaxations, in a 2-layer analysis.[5] An energy minimum at relative displacements of b/3 for sliding between adjacent layers confirms the existence of a twin defect in the present model, where $b$ is the magnitudeof the Burgers vector, $b = a[111]/2$, $a$ being the lattice parameter.

steps. Initially the system responded uniformly, the deformation being elastic and reversible; if the strain were released the system would return precisely to its initial configuration. When the applied strain reached a critical level, the system undergoes a structural transition whereby all the strain in the system is concentrated in the immediate surrounding of the defect, while the other parts of the crystal return to a state of zero strain. The initial and final configurations of such a transition are given in Fig. 6. To visualize the rather complex sequence of atomic rearrangement that must take place, we introduced a simple tiling device to enable us to see the mechanism of the localization process.[11] The tiling procedure consists of imposing a modulating perturbation wave, a sinusoidal wave of negligible amplitude across the system, as shown in Fig. 6. The perturbation is much too weak to have any effect on the dynamical evolution of the system, while the distortion of the wave during localization helps to reveal the local atomic shuffling details that otherwise would be difficult to extract from all the particle displacements in the

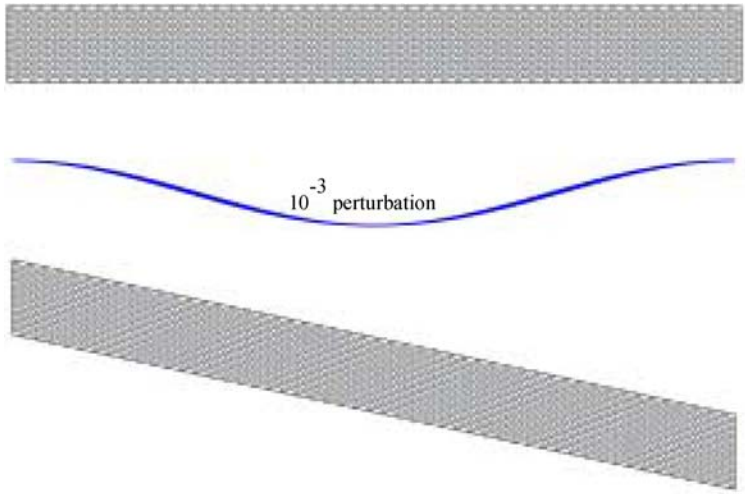


**Fig. 6.** Nucleation of a deformation twin (shear localization), single crystal undeformed (upper) and in final sheared state (lower). Modulating perturbation wave (middle) follows the localization process by virtue of its distortion.

system. The idea is analogous to painting a line across a wall before it starts to collapse and then following how the line breaks up as different parts of the wall start to crumble.

By examining a video of the breakup of the perturbation wave, one is able to describe the sequence of structural transformations occurring in the nucleation of the deformation twin as a 4-stage scenario, which is depicted in Fig. 7. In the initial stage the linear wave grows in amplitude as the applied strain increases. When the amplitude reaches a certain level nonlinearities set in and the wave starts to distort (steepen). As the distortion approaches the critical level the wave front becomes increasingly sharp and collapses into a shock. In the final stage of localization the wave settles into a profile indicating the presence of a twin.

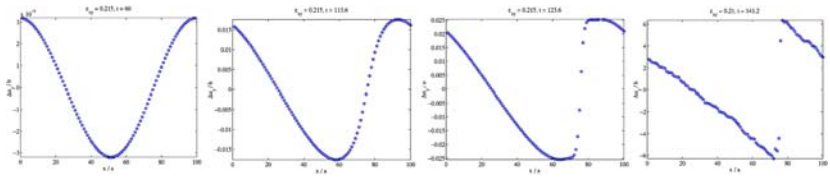

**Fig. 7.** Evolution of the modulating perturbation wave during nucleation of a deformation twin. The wave distortions can be classified in four stages — growth of linear wave, onset of nonlinearity, increasing wave steepening toward a singularity, and final state of strain localization. Wave forms are those of the perturbation wave during the localization event.[12]

## 6. SOFT-MODE SCENARIO

Throughout our discussions we have hinted at a common point of view to rationalize the nature of shear localization in crystals. We see this as fundamental to the understanding of plasticity in crystals, or even more generally local deformation in condensed matter. When the system is driven to a saddle point it will try to go to a local energy minimum nearby. In the event of several accessible minima in the vicinity, then different processes can compete and local kinetic constraints may play a deciding role. Another way to think of instabilities in solids is to recall the concept of soft-mode in lattice dynamics. In the context of lattice vibrations, one may regard the *elastic stability* criteria Eq. (2) as the condition for *vibrational stability* of a crystal lattice in the long wavelength limit. The vanishing of elastic constants then corresponds to phonon modes having vanishing frequency. Indeed one finds such soft modes do occur in a homogeneously strained lattice. Figure 8 depicts the correspondence between the softening of phonon frequencies in a single crystal and the stress-strain response in the same system, both undergoing hydrostatic strain beyond the limit of ideal strength.[14] Dispersion relations, obtained by diagonalizing the dynamical matrix formed numerically, are shown along with a stress-strain curve determined by direct molecular dynamics (MD) simulation using a cell of 4000 atoms at 10 K with periodic boundary conditions. Dispersion curves for the equilibrium lattice are given in the upper left panel, along with neutron scattering data. In the lower panels the system is at the state of critical strain as indicated on the stress-strain curve. The lower left panel shows that phonon modes near the $\Gamma$-point have already become soft.

There is a lattice deformation involving shear localization that is much more extensively investigated than nano-indentation and affine shear. This is the problem of crack tip behavior in a ductile solid. A recent simulation study using reaction pathway sampling has shown that a sharp crack in an fcc lattice, such as Cu, will emit a dislocation loop under critical mode I (uniaxial tension) loading.[15] When the same method is applied to a brittle material, such as Si, a different result is found; the crack front advances by a series of bond breaking and reformation.[16] Thus the deformation response of a solid can be very sensitive to the nature of the chemical bonding. What happens when a relatively brittle material, a semiconductor or a ceramic, is subjected to nano-indentation or affine shear? Preliminary results indicate that the system can undergo local disordering, suggesting yet another competing mechanism of local response to critical stress or strain. Clarification of this kind of phenomenon is work for the future. What hopefully is clear from the present discussion is that informed atomistic simulations will continue to provide a wealth of structural, energetic, and dynamical information about the collective behavior of simple condensed matter, provoking in this way further questions for the statistical-physics community.

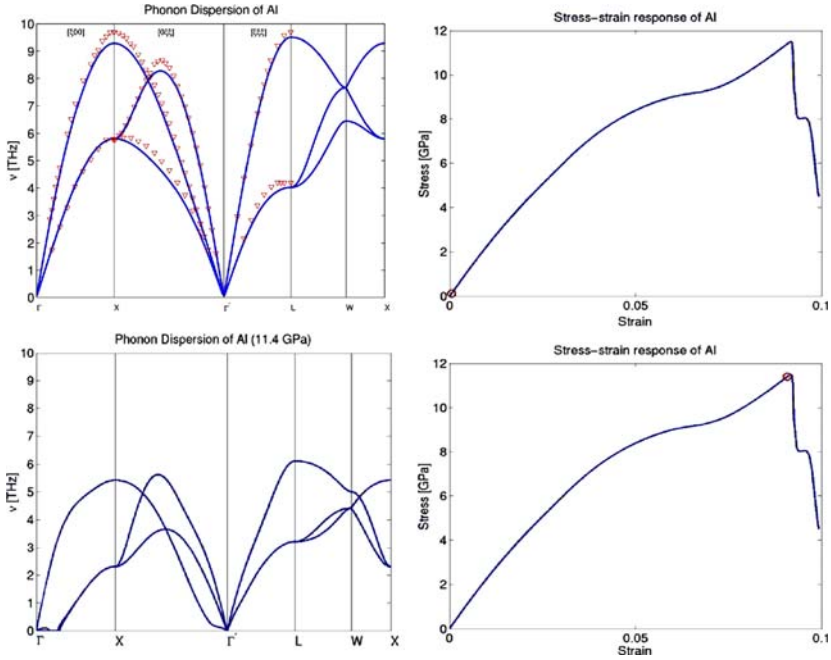


**Fig. 8.** Vibrational response in the form of phonon dispersion curves and stress-strain response of a single crystal under hydrostatic tension.[14] Undeformed results (upper panels) and results in the vicinity of critical strain (low panels), both denoted by the circle on the stress-strain curve. Experimental data from neutron scattering are shown as inverted diamonds.

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