• Review •

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How to identify dislocations in molecular dynamics simulations?^{\dagger}

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Dislocations are of great importance in revealing the underlying mechanisms of deformed solid crystals. With the development of computational facilities and technologies, the observations of dislocations at atomic level through numerical simulations are permitted. Molecular dynamics (MD) simulation suggests itself as a powerful tool for understanding and visualizing the creation of dislocations as well as the evolution of crystal defects. However, the numerical results from the large-scale MD simulations are not very illuminating by themselves and there exist various techniques for analyzing dislocations and the deformed crystal structures. Thus, it is a big challenge for the beginners in this community to choose a proper method to start their investigations. In this review, we summarized and discussed up to twelve existing structure characterization methods in MD simulations of deformed crystal solids. A comprehensive comparison was made between the advantages and disadvantages of these typical techniques. We also examined some of the recent advances in the dynamics of dislocations related to the hydraulic fracturing. It was found that the dislocation emission has a significant effect on the propagation and bifurcation of the crack tip in the hydraulic fracturing.

dislocations, defects, MD simulation, structural characterization, hydraulic fracturing (fracking)

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1 Introduction

Dislocations, which were first described by Volterra [1] in 1907 as topological objects and deeply discussed by Taylor [2], Orowan [3], and Polanyi [4] in 1934, are of key importance in studying the mechanisms of deformed solid crystals [5]. The dislocations could serve as a way for explaining why the theoretical estimates of the ideal elastic limit of perfect crystal by Frenkel [6] give values of 10^3 or 10^4 higher than the lowest observed values [2–4]. Important early milestones in our understanding of the dislocation concept are summarized in Table 1. As typical crystal de-

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fects, dislocations have attracted considerable interests in recent years. Many experimental works [7–11] provided sufficient results to help understand the behaviors of dislocations and other type of crystal defects (e.g., vacancy, interstitial, stacking fault and twinning). Although much progress has been made in experiments, details of defect structures are less well characterized. With the availability of more accurate simulation models and more powerful computing resources, increasingly complex problems in materials science can be addressed and studied at the atomic level [12]. Thus, atomic simulation has been used more extensively to investigate the mechanical properties of crystalline materials [13–18].

MD simulation suggests itself as a natural approach for understanding the intrinsic mechanisms underlying the

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Year	Scientists	Milestone achievements	
1926	Frenkel	theoretical shear strength of ideal crystal	
1934	Taylor, Polanyi and Orowan	crystal dislocations	
1938	Frenkel and Kontorova	speed limit of dislocation motion	
1939	Burgers J M	curved and screw dislocations	
1940	Burgers J M	Burgers vector	
1940	Orowan	Orowan equation for plastic strain rate ^a : $\dot{\varepsilon}_p = \rho_m b V$	
1940	Peierls	Peierls (1940)-Nabarro (1947) stress	
1947	Shockley	partial dislocations and dislocation reactions	
1949	Frank	verification of speed limit of dislocation motion	
1949	Shockley and Read	dislocation model of small angle boundaries	
1950	Peach and Koehler	Peach-Koehler force on dislocation	
1950	Frank and Read	Frank-Read sources of dislocation multiplication	
1956	Burgers brothers	relationship between partial dislocations and stacking fault	
1956	Hirsch and Horne	TEM observation of dislocations	

Table 1 Important early milestones in our understanding of the dislocation concept

a) ρ_m : mean dislocation density; b: Burgers vector; V: dislocation speed.

evolution of crystal defects [19-24]. To the best of our knowledge, the first MD simulation of dislocation was probably proposed by De Wette et al. [25] in 1969. In recent years, lots of MD simulations about dislocations or other crystal defects results have been obtained. For instance, nucleations of partial dislocations were observed during the study of the influence of specimen size on the mechanical behavior of Au pillars by means of MD simulations with the embedded-atom method (EAM) potential by Tang [26,27]. Yang et al. [28] reported that the stresses in the pre-strained nanowires can be released significantly by the dislocation emission from the cascade core when the strain is greater than 1%. In addition, defect formation energies in Cu nanowires have been studied with the classical MD simulations [29]. It was predicted that the vacancy formation energy is the lowest in the middle of the nanowires and the atom formation energy decreases with the decrease of the nanowires diameter. Xu et al. [30] presented a new mechanism that leads to completely healing of nanocracks by the generation of crystal defects known as disclinations without any compressive loads applied normal to the crack faces using MD simulations. Success in these efforts requires simulations and potential functions [31] that are as accurate as possible.

However, the numerical output from the large-scale MD simulations is not very illuminating by itself. To analyze the deformed crystal structure, one is faced with the problem of extracting some relevant information from an enormous set of numerical coordinates. The aim of this paper is to review the typical techniques for detecting the defects in deformed solid crystals, which are routinely adopted in the post-processing of current MD simulations. In this work, the most commonly used structure characterization methods were summarized and discussed in Table 2 and Figure 1.

This paper is organized as follows: in sect. 2, we discussed the typical techniques, which are regularly used in MD simulation to recognize defects, including dislocations, boundaries and point defects, etc. Next, in sect. 3, we briefly described some recent applications to efficiently recognize defects using these methods. Then, the differences between these methods were compared in the sect. 4. In addition, large-scale MD simulations have been carried out to explore the hydraulic fracturing at the atomic scale with the focus on the underlying mechanisms. It was found that the dislocation emission has a significant effect on the propagation and bifurcation of the crack tip, which depends on the impact velocity of the water flow. Finally, we discussed challenges and opportunities of future work in this field.

2 Methods

2.1 Energy or stress filtering

The dislocations can be simply characterized by the distribution of the intensive properties, i.e., the potential energy or the stress. The potential energy or the stress in the region of the crystal with defects is usually higher than that in the perfect region. Thus, the atoms in a certain region where the potential energy or stress is above a threshold are taken as defects. However, this method has limitations in the recognition of defects because of its sensitivity to temperature and force field. Thus, several purely structural analysis methods based on the local atom environment independent of force field have been developed and become the preferred ones in MD simulations [32].

2.2 Atomic local shear strain tensor coloring

For the purpose of quantifying plastic deformation and visualizing defect evolution at the atomic level, the atomic local shear strain [33,34] η_i^{Mises} for each atom *i* is com-

Table 2 The summary of the properties of the typical structure characterization methods

Methods	Advantages	Disadvantages	Applications
energy or stress filtering	simple, universal and no need lattice symmetry	sensitive to temperature	general system
atomic local shear strain tensor coloring [33,34]	powerful, robust and no need lattice symmetry	expensive, a reference configuration re- quired and invalid when large deformation	complex system
local bond order parameters (LBOPs) [36]	independent on crystal orientation	expensive	crystalline and liquid phases
bond angle analysis (BAA) [39]	efficient, robust, able to identify inter- facial atoms and stable against tem- perature boost	difficult to operate	atomic system
coordination number (CN) [35]	easy to implement	sensitive to temperature	metal crystalline
central symmetry parameter (CSP) [40]	efficient and easy to implement	limited to centro-symmetric lattices	centro-symmetric crystal
common neighbor analysis (CNA) [43]	efficient and convenient	unable to identify the interfacial atoms	Metal crystalline, oxide crystalline and semicon- ductor crystalline
adaptive common neighbor analysis (A-CNA) [32]	efficient, convenient and able to identify interfacial atoms	depending on the cutoff radius	multi-phase systems
common neighborhood parameter (CNP) [45]	combination of CSP and CNA	sensitive to structural deformations	metal crystalline, oxide crystalline and semicon- ductor crystalline
Voronoi analysis (VA)	easy extended	expensive, complex, sensitivity to perturba- tions and unable distinguish between fcc and hcp	liquids and glasses
neighbor distance analysis (NDA) [32]	easy to extend and able identify a wide range of coordination structures	expensive	complex system
dislocation extraction algorithm (DXA) [48]	advance and with Burgers vectors can be calculated automatically	complex and need an ideal reference con- figuration	arbitrary lattices



Figure 1 (Color online) Classification of dislocation visualization methods and the software for the post-processing and visualization.

puted, which is also called annotate atomic strain. Calculation of η_i^{Mises} requires two atomic configurations, the current $\{x_i^0\}$ and the reference $\{x_i\}$.

For each neighbor j of atom i, their current separation vector is

$$\boldsymbol{d}_{ji} = \boldsymbol{x}_j - \boldsymbol{x}_i, \qquad (1)$$

and their reference separation is

$$\boldsymbol{d}_{ii}^{0} = \boldsymbol{x}_{i}^{0} - \boldsymbol{x}_{i}^{0}, \qquad (2)$$

where d_{ji} and d_{ji}^0 are all considered to be row vectors. The relative position vector d_{ji}^0 is transformed into d_{ji} by a locally affine transformation tensor J_i . The local Lagrangian strain tensor at atom *i* follows as:

$$\boldsymbol{\eta}_i = \frac{1}{2} \left(\boldsymbol{J}_i^{\mathrm{T}} \boldsymbol{J}_i \cdot \boldsymbol{I} \right), \tag{3}$$

where I is the identify tensor and no summation for i, the observation-frame independent hydrostatic strain invariant is then

$$\eta_i^{\text{hydro}} = \frac{1}{3} \operatorname{tr}(\boldsymbol{\eta}_i), \tag{4}$$

where the trace operation tr() takes the sum of diagonal components in the matrix notation. And the local shear invariant of atom *i* can be computed as:

$$\eta_{i}^{\text{Mises}} = \sqrt{\text{tr}(\boldsymbol{\eta}_{i} - \eta_{i}^{\text{hydro}}\boldsymbol{I})^{2}/2}$$

$$= \sqrt{\eta_{iyz}^{2} + \eta_{ixz}^{2} + \eta_{ixy}^{2} + \frac{(\eta_{iyy} - \eta_{izz})^{2} + (\eta_{ixx} - \eta_{izz})^{2} + (\eta_{ixx} - \eta_{iyy})^{2}}{6}}.$$
(5)

This measure has already been incorporated into the free visualization program AtomEye [35], using standard nearest neighbor cutoff distances for N_i , which is the number of neighbors of atom *i* in the current configuration. This scheme works extremely well in practice [33] for directly visualizing microstructures, including point defects, dislocations, stacking faults, and their strain fields with color encoding.

2.3 Local bond order parameters (LBOPs)

Local bond order parameters (LBOPs) based on spherical harmonics, also known as Steinhardt order parameters [36], are rotationally invariant combinations to determine crystal structures. For a given particle *i*, the *l*-th order parameter follows as [37,38]:

$$q_{l}(i) = \sqrt{\frac{4\pi}{2l+1} \sum_{m=-l}^{l} |q_{lm}(i)|^{2}} , \qquad (6)$$

with

$$q_{lm}(i) = \frac{1}{N_{\rm b}(i)} \sum_{j=1}^{N_{\rm b}(i)} Y_{lm}(\mathbf{r}_{ij}), \qquad (7)$$

where $N_b(i)$ is the total number of nearest neighbor of particle *i*, and *m* is an integer that runs from m = -l to m = l. The functions Y_{lm} are the spherical harmonics and \mathbf{r}_{ij} is the vector from particle *i* to particle *j*. It is important to note that all $q_l(i)$ are rotationally invariant regardless of the choice of *l*.

However, thermal fluctuations smear out the order parameter distributions such that it may be difficult to distinguish between local crystalline structures based on Steinhardt bond order parameters. Then its coarse-grained version including the information of second neighbor shell was introduced as [38]:

$$Q_{l}(i) = \sqrt{\frac{4\pi}{2l+1} \sum_{m=-l}^{l} \left| \overline{q}_{lm}(i) \right|^{2}} , \qquad (8)$$

with

$$\bar{q}_{lm}(i) = \frac{1}{N_{\rm B}(i)} \sum_{k=0}^{N_{\rm B}(i)} q_{lm}(k), \qquad (9)$$

where the sum from k = 0 to $N_{\rm B}(i)$ runs over all neighbors of particle *i* ($N_{\rm B}(i)$ particles) plus the particle *i* itself. Thus, to compute $Q_i(i)$ of particle *i*, one used the local orientational order vectors $q_{lm}(i)$ averaged over particle i and its surroundings. While $q_i(i)$ holds the information of the structure of the first shell around particle *i*, its averaged version $Q_l(i)$ also takes into account the second shell. This spatial averaging added to the standard Steinhardt order parameters has tremendous significance in detecting local ordering with a high sensitivity. Moreover, the values of Q_4 and Q_6 are usually used to discriminate among face-centered cubic (fcc), hexagonal close packing (hcp) and body-centered cubic (bcc) phases. And, in the two dimensional Q_4 - Q_6 - plane, the crystalline structure around a given particle can be characterized by its position. In addition, these LBOPs are often used in computational studies of crystallization to determine the fractions of crystalline and liquid phases.

2.4 Bond angle analysis (BAA)

The bond angle analysis (BAA) is another powerful as well

as robust method for analyzing the crystalline structures obtained from MD simulations, which has been published recently by Ackland and Jones [39]. The BAA method is based on the analysis of angular distribution function of different lattice types and crystal defects. The angular distribution function is described by eight numbers (χ_i), where χ_i is the number of angles in regions of θ_{ijk} chosen to reflect angles actually present in the most likely phases (see Figure 2). Here, θ_{ijk} denotes the angle formed by the given particle *i*, and two of its neighbors, *j* and *k*. Thus, the values of χ_i determined by the N(N-1)/2 bond angle cosines, $\cos \theta_{ijk}$, are calculated first, where N is the number of near neighbors of atom *i*. These neighbors are chosen by a cutoff radius that is proportional to the average distance between the nearest particles and *i*. Then with a heuristic algorithm and series of rules, it is decided which kind of local environment (fcc, bcc, hcp or some other structures) each atom belongs to. Since each structure has a particular angular distribution function, the method enables us to distinguish between fcc and hcp structures even at high temperatures.

2.5 Coordination number (CN)

A coordination number (CN) is defined as the number of nearest neighbor atoms that are within the specified cutoff distance from the central atom. This means that the value of CN can be changed by cutoff control. In a bcc crystal, each interior atom occupies the center of a cube formed by eight neighboring atoms, thus the CN for this structure is 8. Atoms in a perfect bulk fcc crystal have a CN of 12. Atoms with CN less than that of bulk crystal are defined as dislocation or defect cores. In practice, to clearly see the dislocation or defect cores, one needs to remove the perfectly coordinated atoms [35].

2.6 Central symmetry parameter (CSP)

Central symmetry parameter (CSP) is used to characterize the degree of inversion symmetry breaking in each atom's local environment. CSP is defined as [40]:

$$\operatorname{CSP} = \sum_{i=1}^{N/2} \left| \boldsymbol{R}_i - \boldsymbol{R}_{i+N/2} \right|^2, \qquad (10)$$



Figure 2 (Color online) The illustration of the distribution of χ_i and the value of the χ_i for ideal bcc, fcc and hcp. Note that the void is zero.

where the *N* nearest neighbors of each atom are identified. We may want to use N = 12 or 8 for fcc and bcc lattice, respectively. \mathbf{R}_i and $\mathbf{R}_{i+N/2}$ are vectors from the central atom to a particular pair of nearest neighbors. N(N-1)/2 possible neighbor pairs could contribute to eq. (10). The quantity in the sum is computed for every pair, however only the N/2 smallest are actually used, which are typically the pairs of atoms in symmetrically opposite positions with respect to the central atom [41].

From eq. (10), we could deduce that for an atom on a perfect lattice, the CSP will be 0. It will be approach to 0 for small thermal perturbations of a perfect lattice. If a point defect exists, the symmetry is broken, and the parameter will be a larger positive value. An atom at a surface will have a large positive parameter [42]. Consequently, CSP is a useful measure of the local lattice disorder around an atom and can be used to characterize whether the atom is part of a perfect lattice, a local defect (e.g., a dislocation or stacking fault), or at a surface [41]. Especially, CSP is also useful for visualizing planar faults in fcc and bcc crystals [40].

2.7 Common neighbor analysis (CNA)

Another popular structure analysis method for dislocation visualization is the common neighbor analysis (CNA), which was proposed by Honeycutt and Andersen [43]. In solid-state systems, the CNA pattern is a useful measure of the local crystal structure around an atom. In CNA method, a characteristic signature is computed from the topology of bonds that connect the surrounding neighbor atoms [32]. In contrast, CSP method directly considers the spatial vectors which point from a given atom to its neighbors. The CNA methodology was described in detail by Faken, Tsuzuki and their coworkers [44,45]. CNA uses the local crystal structure which is represented by diagrams to find defects. The diagram is classified in the following way: A set of four indexes: i, j, k, and l are used to classify the diagram. The first index, *i*, indicates the diagram "type". If a pair of atoms, α and β are near-neighbors, then i = 1, otherwise, i = 2. The second index, j, represents the number of near-neighbors shared by the (α, β) pair, which means the common neighbors. The third index, k, indicates the number of bonds between these common neighbors. The forth index, l, differentiates diagrams with same i, j, and k indexes and different bonding between the common neighbors [45]. There is a slight difference between Tsuzuki's CNA parameters and the CNA indexes proposed by Faken et al. [44]. The latter has only three indexes. In LAMMPS [41] and OVITO [46], fcc, hcp and bcc crystals are encoded as integer values 1, 2, 3, respectively. Note that CNA is confused by thermal vibrations, for that reason it is a good idea to run CNA on thermally averaged positions.

2.8 Adaptive common neighbor analysis (A-CNA)

In CNA method, we used the cutoff radius to determine the

nearest neighbors. In some case it is difficult to choose this cutoff radius correctly, in particular multiphase systems, hence an adaptive version of the CNA has been developed that works without a fixed cutoff radius. This adaptive common neighbor analysis (A-CNA) method determines the optimal cutoff radius automatically for each individual particle [32]. Considering the atoms just at the interface, the CNA method can not assign a structural type, because the corresponding coordination does not match to either of the reference structures. The A-CNA method can overcome this problem. It computes each atom's cutoff radius and considers the local dilatation. The A-CNA method is a simple extension of the standard CNA method, which adds the ability to analyze multi-phase systems and some convenience on the user's side [32].

2.9 Common neighborhood parameter (CNP)

Combining of the CSP and CNA methods, the definition of the common neighborhood parameter (CNP) can be obtained [45]. The definition follows

$$CNP = \frac{1}{n_i} \sum_{j=1}^{n_i} \left| \sum_{k=1}^{n_j} \left(\boldsymbol{R}_{ik} + \boldsymbol{R}_{jk} \right) \right|^2, \qquad (11)$$

where \mathbf{R}_{ik} indicates the vector connecting atom *i* to atom *k*. Note that the index *j* goes over the n_i nearest neighbors of atom *i*, and the index *k* goes over the n_{ij} common nearest neighbors between atom *i* and atom *j*. For perfect fcc and bcc crystals, CNP = 0.

2.10 Voronoi analysis (VA)

In the Voronoi decomposition, the characteristic arrangement of near neighbors of a particle can be reflected by the geometric shape of the Voronoi polyhedron. Consequently, the Voronoi analysis (VA) has been used in many MD simulations to analyze dislocation dynamics [47].

By counting the number of polygonal facets having three, four, five and six vertices/edges, the computed Voronoi polyhedron for a particle is translated into a compact signature in this method. This yields a vector of four integers further identifying the structural type [45]. For instance, the corresponding signature of an fcc lattice is (0, 12, 0, 0)while that of a bcc lattice is (0, 6, 0, 8).

2.11 Neighbor distance analysis (NDA)

Neighbor distance analysis (NDA) [32] method is based on an identifier, using the coordinates of a particle, which is rotationally invariant and can be easily compared. Unlike the CSP, it does not require special ordination of the particles or the pre-existence of certain conditions of symmetry.

The near distance $d_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ between two neighbors *i* and *j* of a given particle is compared with the reference pattern

adjusted with a small margin causing by the elastic distortions of an actual crystal or thermal vibration for all N(N-1)/2 neighbor pairs of the given particle in this method. Note that d_{ij} is invariant under rotation. The test structure is considered not match the reference pattern if any of the distances falls outside the corresponding admissible range. Here, N, which is the number of nearest neighbors to be taken into account, should include complete shells and be as small as possible for best efficiency. The increased computational cost of the NDA makes it only be recommended in the case of structures that have not been identified by another analysis method easier.

2.12 Dislocation extraction algorithm (DXA)

The dislocation extraction algorithm (DXA) was proposed by Stukowski and Albe [48], which is a general and powerful method for characterizing the topological structure of dislocations from atomic simulations. It converts identified dislocation networks into continuous lines and determines their Burgers vectors in a fully automated fashion even in highly distorted crystal regions. As the first step of this method, the dislocation core atoms are characterized through the standard CNA method. Then, an oriented, closed, two-dimensional manifold called interface mesh is built. It distinguishes the crystalline atoms from the disordered ones. Finally, on this manifold for each dislocation segment, an initial Burgers circuit is constructed (Figure 3). While the closed Burgers circuit and its reverse copy are swept in both directions, a one-dimensional line representing of the dislocation segment is obtained by recording the current mass center of the Burgers circuit and the Burgers vector can be computed.

However, the above description of the DXA is limited to perfect lattice dislocations in the fcc and bcc lattices. Thus, the extended version of the DXA was developed by Stukowski et al. [49], which can identify and index dislocations



Figure 3 (Color online) Schematic of the DXA. First a manifold surface enclosing the dislocation cores is constructed. Then elastic "Burgers circuit bands" are swept over the manifold along each dislocation segment. Finally, nodal points are generated where multiple Burgers circuits meet on the manifold [48].

including partial dislocations and secondary grain boundary dislocations and determine their Burgers vectors in arbitrary crystalline model structure and coherent crystal interfaces. In this recognition, the incompatible elastic displacement field induced by dislocations is computed by mapping atomic bonds from the distorted atomic configuration to an ideal reference configuration. An atomic structure identification algorithm and a set of ideal templates are used to locally determine the reference configuration. The ideal templates include the perfect lattices, the coherent crystal interfaces and the ideal stacking faults. The algorithmic steps are illustrated in Figure 4. Therefore, the extended version of the DXA provides a robust and simple-to-use method for automatically detecting any such dislocations in atomic configurations, computing the Burgers vectors, and representing arbitrary dislocation networks by connected and fully indexed lines. It is a useful tool to analyze and visualize atomic simulations of crystal plasticity.

3 Applications

3.1 Energy filtering

In the research of purely stress-driven interactions between non-screw lattice dislocation and coherent twin boundary (CTB), the energy filtering technique was used to recognize the defective atomic structures. With the atoms colored with potential energy, MD snapshots (Figure 5) illustrate that the dissociated dislocation recombines into a perfect dislocation configuration at the CTB and then cuts through the boundary by splitting into three Shockley partials. However, the



Figure 4 (Color online) Illustration of the generalized DXA. In this example, a prismatic dislocation loop in a bcc single crystal is identified, indexed and converted to a continuous line representation [49].



Figure 5 (Color online) MD snapshots illustrating interaction between an incoming dislocation and the CTB in Cu [54].

atomic energy levels of perfect lattice atoms and metastable defects can easily overlap due to degeneracies, elastic strain energy or thermal energy. As a consequence, this method is generally not the first option nowadays.

3.2 Atomic local shear strain tensor coloring

The atomic local shear strain tensor coloring is a good measure of local inelastic deformation. For the circular cross-sectional silicon nanowire under compressive loading, the snapshot of the deformation reveals that the first slip event is initiated by the nucleation of a dislocation half loop from the surface and propagates in $(0\overline{11})$ direction [19]. With the atoms colored with atomic local shear strain tensor, the mechanism of the deformation can be observed in Figure 6.

3.3 Coordination number (CN)

MD simulation of spherical indentation normal to the $\langle 111 \rangle$ surface of Al shows the atomic-level details of dislocation nucleation and subsequent incipient plasticity [50]. With the atoms colored by CN, the nucleation and propagation of dislocations can be clearly captured. As shown in Figure 7, a sessile structure derives from homogenously nucleated glide loops on three equivalent {111} planes. In addition, dislocation half-loops on two {111} $\langle 110 \rangle$ slip systems cross-slip and pinch off from the metal surface, forming a prismatic dislocation loop which moves through the crystal.

3.4 Local bond order parameters (LBOPs)

LBOPs were successfully applied to disclose the dislocation structures evolution in nanocrystalline metals [51]. As shown in Figure 8, atoms are colored with local crystal



Figure 6 Atomic local shear strain tensor coloring shows the dislocation propagation in compressed silicon nanowire. No nucleation of dislocation is shown at low strain in (a). As strain increase further, dislocation nucleates at the surface in (b) and propagates along the $(01\overline{1})$ plane in (c)–(e), eventually creating a surface step in (f). The atoms are colored by the atomic local shear strain [19].



Figure 7 Homogeneous defect nucleation in (111) spherical indentation of Al [50].

order and the snapshots show that plastic deformation is dominated by partial dislocations gliding parallel to twin planes in Figure 8(a) with twin boundary spacing of 1.25 nm, whereas dislocations cutting across twin planes is the controlling deformation mechanism in Figure 8(b) with twin boundary spacing of 6.25 nm. This coloring technique is extremely helpful to understand the deformation mechanisms of nanocrystals.

3.5 Bond angle analysis (BAA)

The BAA method is efficient for distinguishing fcc, hcp and bcc coordination structures. In MD simulations of mechanical behaviors of irradiated metal nanowires, this technique is adopted to trace the interaction between dislocation and their defects [28]. Upon tensile loading of the Cu nanowire with a 10 keV irradiation, as shown in Figure 9, the first leading partial dislocation is nucleated from the dislocation loop induced by the irradiation and moves around the nucleation site anticlockwise and forms a stacking fault across the nanowire section. After that, a trailing partial dislocation is emitted from the same site and moves around the "pin" in counter-clockwise direction and finally moves out of the nanowire. The "pin" effects of the defect cluster on the dislocation may attribute to the strain hardening behavior.

3.6 Central symmetry parameter (CSP)

Atomic modeling was performed to understand the mechanisms of the ultrahigh strength and high ductility of nano-



Figure 8 Simulated deformation patterns in nano-twinned samples with different twin boundary spacing five types of atoms are painted in color: grey for perfect atoms, red for atoms in stacking faults and green for atoms in grain boundaries or dislocation cores; blue atoms indicate that they are in the vicinity of vacancies; and fully disordered atoms are yellow [51].



Figure 9 (Color online) The incipient plastic deformation of the nanowire after a 10-keV ion irradiation then subjected to tensile loading. Leading partial "L" nucleates at the elastic limit (a), then propagates from (b) to (c), where leading partial moves around the "pin". The dislocation is absorbed by surface at (d) and trailing partial "T" nucleates at the cascade core. Approximate circular motion of trailing partial "T" can be observed from (e) to (g), and finally moving out of the nanowire (h), leaving only defect clusters in the nanowire [28].

twinned copper [52]. With the atoms colored by the CSP, the stacking fault and TB can be indicated. By the snap of the evolution of the atomic structure, two competing pathways are identified. Atomic modeling of interface-mediated slip transfer reactions shows atomic configurations of absorption, desorption and direct transmission, as shown in Figure 10.

3.7 Common neighbor analysis (CNA) for hydraulic fracturing simulations

Hydraulic fracturing, which leads to the booming of shale gas, is an important modern technique for extracting the shale gas from the shale rock with numerous nanometer pores by creating extensive artificial fractures. In this work, large-scale MD simulations have been carried out to explore the hydraulic fracturing at the atomic scale with the focus on the underlying mechanisms. To simplify the simulations, we used the Lennard-Jones (LJ) substrate with fcc crystal structure to model the shale. And the extended simple point charge (SPC/E) water model was used to describe the intermolecular interactions between water molecules. The whole system was modeled in micro-canonical ensemble (NVE) with a step of 1 fs. An initial crack tip was preset in the shale. The water flow was given a certain macroscopic velocity to exert hydraulic pressure to the shale. And the hydraulic pressure was controlled by the velocity of the water flow. It was found that different impact velocities of the water flow lead to different kinds of cracks in our simulations. When the impact velocity is lower than 0.428 times

Rayleigh surface wave speed, the water flow can only induce one crack, whose propagation is not along a straight line, but turns a corner in the end. When the impact velocity is about 0.472 times Rayleigh surface wave speed, the propagation of the crack tip becomes unstable under the impact of the water flow. The crack bifurcates, i.e., forming two cracks, which propagate along different directions. And further increase of the impact velocity could even lead to the formation of three cracks, which propagate along different directions (Figure 11). Figure 12 shows the dislocations evolutions of the fcc crystal under the impact of the water flow using the CNA methods. With the increase of the pressure, the dislocations nucleate firstly at the crack tip and the points with stress concentration at the left and the right edges. A group of parallel partial dislocations emit from the cores and then slip on (111) and $(11\overline{1})$ planes, leading a set of parallel stack faults behind. Two triangular areas are formed after the dislocations slipping, with very high density of stack faults. The dislocations from the two edges finally interact with the dislocations emitted from the bifurcate crack tips till the complete disintegration of the material.

In summary, the atomic details of hydraulic fracturing were shown through the MD simulations. First, we found that the bifurcation of the crack tip depends on the impact velocity of the water flow. Second, it was found that the dislocation emission has a significant influence on the bifurcation and propagation of the crack tip [53]. Our findings and related analysis may help uncover mechanisms of hydraulic fracturing.



Figure 10 (Color online) Atomic configurations of (a) absorption, (b) desorption and (c) direct transmission, respectively [52].



Figure 11 (Color online) The bifurcation of the crack tip in the hydraulic fracturing. Note that c_{tip} is the critical crack tip velocity and c_R is the Rayleigh surface wave speed. (a) $c_{tip}\approx 0.428c_R$; (b) $c_{tip}\approx 0.472c_R$; (c) $c_{tip}\approx 0.503c_R$.



Figure 12 (Color online) The dislocations propagation in hydraulic fracturing using the CNA methods. (a)–(i) The evolution of the dislocations and the stacking faults of the fcc crystal under the impact of the water flow; (j) the locally zoom version of the picture (f). All perfect crystal atoms are suppressed for clarity.

4 Comparisons

In solid-state systems, the CSP is a useful measure of the

local lattice disorder around an atom. A large number of researches have proved that the CSP coloring can be used in MD post-processing for characterizing whether the atom is part of a perfect lattice, a surface or a local defect (e.g., a dislocation or stacking fault). However, to compute CSP, the neighbor list needs to be constructed. Thus, it is unable efficiently compute this quantity too frequently.

Another useful measure of the local crystal structure is the CNA pattern, which is sensitive to the specified cutoff value. The appropriate nearest neighbors of an atom should be found within the cutoff distance for the tested crystal structure (e.g., 14 nearest neighbors for perfect bcc crystals and 12 nearest neighbor for perfect fcc and hcp crystals). The accuracy of CNA depending primarily on reliable identification of the neighbors is similar to BAA. In contrast to the CSP, BAA is more stable against temperature boost, since it is based on the angles but not the distance between particles. Therefore statistical fluctuations are averaged out a little more.

A CN is defined as the number of neighbor atoms with specified atom types that are within the specified cutoff distance from the central atom. Atoms not in the group are included when computing the coordination number of atoms in that group.

The atomic local strain tensor coloring is originally proposed by Shimizu et al. [33], which is different from the von Mises shear strain invariant coloring in which two configurations are required, one current and one reference configuration. It is also much more powerful and robust than the former because it does not rely on assumptions of prior high lattice symmetry.

5 Conclusions

Scientific data analysis is essential to understand the science under a certain physical phenomena. The aim of this paper is to review the typical techniques for detecting the defects in the deformed solid crystals, which are routinely adopted in the post-processing of current MD simulations. Datasets produced by MD simulations are often very large, which results in a time-consuming data analysis. Retrieving useful information and drawing conclusions from such a large-scale simulation requires reliable methods to recognize defects efficiently. Some efficient methods, such as CNA, CSP and LBOPs, have been developed to visualize and interpret the defects (e.g., vacancy, interstitial, dislocation, stacking fault and twinning) in all kinds of solid crystals. Based on the comparison of the available techniques, the above mentioned methods of structure identification show their merits and also have limitations in recognition of defects at high temperature or under large deformation. For the complex systems, combination of the techniques may be needed.

Previous researches have proved these techniques can not

only disclose fundamental mechanisms of defects nucleation and growth processes but also provide essential evidence of softening or strengthening of materials [55]. Furthermore, several key issues should be addressed in future work, such as identification of complex lattices, lattices with strong thermal perturbation and large deformed lattices. In addition, more universal, efficient, convenient and intuitive method would be applied to obtain the dislocations and other type of defects without complex analysis by users in the future.

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