Atomistic simulations of incipient plasticity under Al(111) nanoindentation

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Abstract

Atomistic simulations are performed for the study of defect nucleation and evolution in Al single crystal under nanoindentation. Methodologies employed include the molecular dynamics and molecular mechanics simulations with embedded-atom potentials. Simulated is the indenting process on Al(111) surface with the spherical tip of indenter. Using the visualization technique of centrosymmetry parameters, homogeneous nucleations and early evolutions of dislocations are investigated for deepening our understanding of incipient plasticity at the atomic scale. We have shown that the nucleation sites of initial dislocation loops vary with the empirical potentials chosen for the simulation. Identifications are also made for the continuously changing structures of dislocation locks underneath the indenter tip and for the glide of prismatic partial dislocation loops far away from the contact surface.

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1. Introduction

Modelling and simulation of material behaviors at the nanoscale have recently been attracting much attention in computational solid mechanics (Needleman, 2000; Kouris and Gao, 2002; Liu et al., 2004b). In particular, with the advent of atomic force microscopy, direct molecular dynamics and molecular mechanics simulations of nanoindentation-induced defect mechanism have become popular models to explore for the better understanding of the atomic-level mechanism of plastic deformation. For example, from their atomistic simulations of nanoindentation, Kelchner et al. (1998) found that initial partial dislocation loops were nucleated off the indenting axis below the Au(111) surface. Li et al. (2002) and Van Vliet et al. (2003) performed molecular
dynamics simulations of Cu(111) and Al(111) nanoindentations for the comprehensive study of dislocation nucleation and kinetics. Using energy minimization and constant-temperature molecular dynamics, Rodriguez de la Fuente et al. (2002) demonstrated the formation and movement of hillocks on Au(001) surface under nanoindentation. Investigations on the defect evolution when indenting face-centered cubic (fcc) (001) surface were also presented by Gannepalli and Mallapragada (2002). As well as fcc single crystals, defect generation mechanisms in indenting crystal surfaces of other lattice structures have been studied, such as Fe single crystal by Smith et al. (2003) and Si(001) surface by Gannepalli and Mallapragada (2001). The effects of grain boundary on defect formation when indenting bi- and poly-crystals have moreover been examined through atomistic simulations by Feichtinger et al. (2003) and Lilleodden et al. (2003).

In addition to the understanding of defect mechanism at the nanoscale, the atomistic simulation of nanoindentation-induced plastic deformation provides theoretical foundation for establishing the hierarchical modelling of material defects across different length scales, each of which is based on the independent framework of physics such as quantum, atomic, and continuum physics. As a part of the hierarchical modelling of plasticity, direct atomistic simulation occupies a particularly important position because they are to be combined simultaneously with the two distinctive recognitions of plastic deformation: the electronic origin of dislocation nucleation based on quantum physics, and the continuum-based mesoscale approach of multiple-dislocation cooperations and interactions. Atomic-level numerical simulations with empirical interatomic potentials are practically indispensable for lessening the enormous computing load due to first-principles calculations. They further serve as atomic-resolution evidences of the macroscopic continuum-based quantities that can be observed in actual nanoscale experiments generating defects in materials. For instance, Zhu et al. (2004) has most recently proposed an energy-based local elastic stability criterion with atomically informed continuum quantities in order to accurately predict homogeneous dislocation nucleations in Cu(111) nanoindentation. They evaluated their theoretical prediction by comparing with direct molecular dynamics simulations of the same example. Therefore, understanding the defect mechanism at the atomic scale through accurate modelling and simulation is an essential premise to achieve progress in the hierarchical materials modelling without any information leakage across scales.

In this work, using both conjugate-gradient energy minimization and molecular dynamics, we perform the simulations of nanoindentation on Al(111) surfaces for the atomic-level analysis of incipient plasticity. A general perspective on the typical mechanism of defect generation and evolution underneath the indenter tip is presented with detailed investigations of representative stages among the whole deformation procedure. Included are the embryonic and tetrahedral dislocation locks at the earliest stage, complex local glides of dislocation loops at the intermediate step, and the glide of a prismatic partial dislocation loop mediating permanent deformation far away from the contact surface. Structural identifications of those defects are also provided. Meanwhile, the focus of this work is laid on the homogeneous nucleation of dislocation, in comparison with the above mentioned $K$ criterion by Zhu et al. (2004) and other atomistic simulation results of fcc(111) nanoindentation reported in the literature. We demonstrate that, in some cases, the sites of homogeneous dislocation nucleation obtained from our simulations are not completely consistent with the ones predicted by the $K$ criterion. Subsequently it is evidenced that the disagreement is caused by the different empirical interatomic potentials employed. Discussions on our simulation results are thus expected to be beneficial for enlarging our understanding of plastic deformation at the nanoscale.

This paper is outlined as follows. Section 2 introduces the simulation methodologies employed for this work including empirical potentials, indenter tip modelling, temperature and boundary conditions, and visualization techniques. A general overview of typically observed defect structures and their motions under Al(111) nanoindentation is presented in Section 3. Next, Section 4 begins
with investigating the homogeneous nucleation of dislocations and comparing our results with others reported elsewhere. The rest of Section 4 is then devoted to the identifying analysis of other defects subsequently generated and developed following the initial dislocations. Finally the concluding remarks involving future prospects are given in Section 5.

2. Simulation methodology

Classical molecular dynamics (MD) simulation is in principle to solve numerically the Hamilton’s equation of motion for each atom (or molecule) with respect to time (Allen and Tildesley, 1987; Frenkel and Smit, 2001; Rapaport, 1997). For the time-marching method in our simulations, we employed the velocity Verlet algorithm with the single time step of 5 (fs). Intertatomic interactions in classical MD simulations are generally represented by empirical potentials chosen appropriately for the atomic system considered. The embedded-atom method (EAM) potential is the most popular one used for fcc crystals such as Cu, Au, Ag, and Al. Among many different types of EAM potentials, we used the EAM glue potential for most examples of this paper. This potential was proposed by Ercolessi and Adams (1994) and has been known to be accurate especially for Al surfaces. Numerous molecular dynamics studies of deformation processes in Al have been performed using the Ercolessi–Adams glue potential, as in Yamakov et al. (2002) for example. The glue potential has also been applied for the recent nanoindentation simulations of Al single crystal by Yip and coworkers (Li et al., 2002; Van Vliet et al., 2003). For the comparative study of a specific example of homogeneous dislocation nucleation, we further simulated the nanoindentation with two other EAM potentials suggested by Cai and Ye (1996) and by Mishin et al. (1999, 2001) respectively.

Our attention in this work focuses on the defect mechanism inside Al substrate, rather than the interaction between the indenter tip and surface atoms. Therefore, as popularly used for MD nanoindentation simulations, the interaction between the indenter tip and Al atoms is here modelled through a simple repulsive potential, instead of describing the tip by a cluster of realistic atoms (Kelchner et al., 1998; Li et al., 2002; Van Vliet et al., 2003; Zhu et al., 2004). This numerical model of indenter tip, is effective especially for the atomistic simulation of nanoindentation on passivated surfaces as mentioned by Kelchner et al. (1998) and Gannepalli and Mallapragada (2002). The repulsive potential of indenter tip, as in Li et al. (2002), is here used as

\[
V_{\text{tip}}(r) = \begin{cases} 
\exp \left( \frac{d-r}{d} - \frac{R-r}{R} \right), & r < R \\
0, & r \geq R
\end{cases}
\]

(1)

where \(d\) is a parameter controlling the hardness of indenter tip. Throughout this work, it is set \(d = 0.12\) (nm). \(r\) denotes the atom’s distance from the center of the spherical indenter tip of which the radius, \(R\), of 5 (nm) is here used for all our numerical experiments.

In this paper, we restrict our simulations within the mechanical study of defects, not considering the full effects of temperature on defect generations and movements. We have thus set the target temperature 1 (K) by continuously re-scaling the velocity with the thermostat proposed by Berendsen (1984). Its re-scaling parameter, \(\lambda\), to be multiplied to the atom’s velocity at each time step, is defined as

\[
\lambda = \left[ 1 + \frac{\Delta t}{\tau_T} \left( \frac{T_0}{T} - 1 \right) \right]^{1/2}
\]

(2)

where \(\Delta t\), \(T_0\), \(T\), and \(\tau_T\) are the single time step, the target temperature, the current temperature, and the temperature-coupling time constant of the system, respectively. Using the constant \(\tau_T\), we are able to control how quickly the current system converges to the target temperature. The temperature-coupling time constant is here set 1000 times greater than the single time step of our time-marching algorithm. This value cools the system down to the target temperature so adequately that the unintended thermal activation of defect and the undesirable wave reflection from boundaries be minimized during simulation process, as proposed by Van Vliet et al. (2003). Due to the limitation of computing power, the speeds of indenter...
tip reported in the references are an order of 1–100 (m/s) for most molecular dynamics simulations of nanoindentation. It is surely too high to be realistic and to reproduce the actual experiments of quasi-static indenting course. In our simulation as well, the indenting speed is fixed 10 (m/s). The above value of temperature-coupling time constant $\tau_T$ is thus highly useful also in minimizing the unrealistic effects raised by this extremely high speed of the indenter tip.

An example of models for our nanoindentation simulations is shown in Fig. 1, which contains 1,512,000 Al atoms in the domain of 34.2 (nm) $\times$ 34.6 (nm) $\times$ 21.0 (nm). The largest model used in this paper is 37.6 (nm) $\times$ 38.0 (nm) $\times$ 23.0 (nm) of 2,012,472 atoms while several different sizes of domain were simulated for case studies. As shown in Fig. 1, the surface indented is (111) for all the numerical experiments in this paper. We prescribe the periodic boundary conditions on the four sides of the simulation domain, while free boundary conditions are imposed on the top and bottom surfaces. Due to the free boundary of the bottom, dislocation loops, being emitted from the under-the-tip region and gliding downward, do not bounce back from the bottom surface and thus they do not have any chance to deteriorate our observation underneath the indenter tip. Instead, the loop disappears out leaving a parallelogram surface step on the bottom. Detailed description on the glide of a prismatic dislocation loop will be given in the following section. In order to prevent the whole domain from being translated downward due to the force applied by the indenter tip, we first divide the same amount of the force by the total number of atoms in the model, and then allocate the resultant, as a part of externally applied force, equally to each of the Al atoms in the opposite direction. This technique has been adopted by Li et al. (2002) and Van Vliet et al. (2003). Consequently, this pseudo body force maintains the model, as a whole, to be in neither translational nor rotational motion.

One of the most important ingredients in the atomistic simulation of defect nucleation and evolution is the technique to selectively visualize interior defects. We employed the visualization technique of centrosymmetry parameter that has successfully proven effective for the studies of dislocation nucleation in fcc crystals by Kelchner et al. (1998) and Lilleodden et al. (2003). Every atom in perfect fcc single crystal has twelve nearest-neighboring atoms. Each of the neighbors can be paired with an opposite nearest neighbor. The centrosymmetry parameter, $P$, is then defined as

$$P = \sum_{i=1}^{6} | R_i + R_{i+6} |^2$$

where the $R_i$ and $R_{i+6}$ together stand for the six pairs. The parameter therefore vanishes for each atom that rests at the site of perfect fcc lattice structure. If there exists a defect such as vacancy and dislocation, the parameter for an atom in the vicinity of the defect has some finite magnitude much greater than that caused by the local atomic

![Fig. 1. An example of simulation models for Al(111) nanoindentation.](image)
vibration around each fcc site. When its magnitude is less than a cutoff value, we eliminated the corresponding atom from visualizing our simulation results. Therefore, only defect-related atoms are visible along with those at the non-periodic boundaries. The cutoff value used is adequately selected to be 0.01, after making the parameter dimensionless through dividing it by $\frac{1}{\langle \rho \rangle}$. With this help of centrosymmetry parameter technique, we were able to visualize not only point defects but also dislocations and stacking faults, for the comprehensive analysis of incipient plasticity under nanoindentation. For a graphical tool, we utilized the open software, AtomEye, developed by Li (2003).

3. An overall procedure of incipient plasticity under Al(111) nanoindentation

In this section, we present the general description of typical deformation procedure observed when indenting Al(111) surface. The whole procedure considered here is up to the emission of an isolated prismatic partial dislocation loop traveling downward to the bottom surface, because this glide implies the very first permanent deformation transmitted along its path far away from the local contact zone. Only a brief summary is given in this section because our intention is to provide beforehand the general idea of defect evolutions occurring underneath the contact surface. Detailed analysis of each deformation stage of note and the corresponding defect structure will be considered in the following section.

Fig. 2 shows the load–displacement curve obtained from the simulation of the model comprising 2,012,472 atoms. The load in the figure is defined as the summation of vertical components of the repulsive forces calculated from the tip potential given by Eq. (1). The displacement means the penetration depth from the first contact point on the indented Al(111) surface. In Fig. 2, (i)–(v) depict distinctive durations separated by (α)–(δ). The instants (or extremely short durations) marked by (α)–(δ) respectively represent the significant changes in deformation or defect structure that are instantaneously taken place. During the section of (i) prior to the first load relaxation at (α), the deformation is elastic. The nucleation of initial defect beneath the tip is observed at the instant of (α) and the well-known dislocation embryos are immediately developed from the sites of homogeneous nucleation, as resulted in the prospective close-up view of Fig. 3(a). Note that the atoms in perfect fcc configuration are all eliminated in this visualization by centrosymmetry parameter. Those embryonic dislocations maintain their shape all through the stage (ii), until it is transformed into the tetrahedral sessile lock of Fig. 3(b) at the second major load relaxation of (β) in Fig. 2.

Throughout the period (iii), any substantial changes of defect structure are not found, except local glides of partial dislocation loops emanating from the faces of tetrahedron. These dislocation loops keep competing to grow until one of the candidates is finally triggered to evolve into an isolated prismatic partial dislocation loop around the moment of (γ). The load–displacement curve during this period of competition is oscillatory due to the complex local motions of dislocations beneath the tip, but it still results in overall increase of load response. The accumulated energy is thus released partly through the growth of a
prismatic partial dislocation loop to be emitted. However, it is almost impossible to predict precisely when the prismatic loop is emitted because of the instability nature all over the procedure. For example, we have simulated the same indentation example with a smaller domain size of $34.2 \times 34.6 \times 21.0$ (nm) which involves 1,512,000 Al atoms. The first emission of prismatic loop occurs much later than the case of the above larger model. It is because, in this smaller case, two local dislocation loops happen to separately grow into partial dislocation loops in parallel for a long time just before the first emission. This long-lasting growth competition between dislocation loops absorbs considerable amount of energy and thus sustains the increasing load without any emission of prismatic dislocation loop. Fig. 4 illustrates four snapshots of an isolated loop development process, accompanying gentle load drop during the corresponding stage of (iv).

After being separated from the local zone of defect at (d), this partial dislocation loop at last begins its long glide through the thickness downward to the bottom surface as given in Fig. 5. Note again the attribute of current visualization technique. Atoms are simply vibrating around their sites. In Fig. 5, what is gliding through is therefore not a specific atom itself but the local imperfection of fcc atomic configuration, such as propagating waves. As can be seen in the figure, the prismatic loop disappears to leave a surface step on the bottom, which is the evidence of permanent deformation mediated through the glide. The energy release due to the emission of dislocation loop, leads to the overall re-increase of indenting load during this period of glide until the second partial loop is triggered to fully grow, as denoted by (v) in Fig. 2.

4. Analysis of significant stages in nanoindentation-induced defect evolution

Briefly sketched in the preceding section is the whole procedure of incipient plasticity that is typically observed inside the material when indenting Al(111) surface. With this general idea of deformation process, we further analyze our simulation results in this section. Among the deformation sequence, we here select three significant stages to investigate in more detail to better comprehend the mechanism of incipient plasticity in Al(111) nanoindentation. They are the homogeneous dislocation nucleation and subsequent embryonic dislocation loops, the tetrahedral sessile lock with local glides of competing dislocations, and the long glide of an isolated prismatic dislocation loop.

4.1. Homogeneous nucleation of dislocation

Recent years have witnessed increasing interests in atomically resolved predictions of the onset of plastic deformation specifically induced by nanoindentation (Chen et al., 2003; Corcoran et al.,
Interesting results have thus far been revealed by direct atomic simulations, in cooperation with experiments, of nanoindentation. One of the notable findings reported is that, when indenting fcc(111) surfaces, the nucleation sites of dislocations beneath the tip are displaced from the indenting axis, as demonstrated in the simulations of nanoindentation of, e.g., Au(111) by Kelchner et al. (1998) and Lilleodden et al. (2003), Al(111) by Van Vliet et al. (2003), and Cu(111) by Zhu et al. (2004). It is therefore admitted that the critical resolved shear stress (CRSS) criterion based on continuum elasticity theory is no longer valid in predicting the homogeneous nucleation at the atomic resolution under the nanoindentation of fcc crystals. This failure of CRSS criterion recently motivated Yip and coworkers (Li et al., 2002; Van Vliet et al., 2003; Zhu et al., 2004) to develop an energy-based local elastic stability criterion, named \( K \) criterion, for the accurate prediction of nanoindentation-induced homogeneous dislocation nucleation. The criterion was formulated with physical quantities of continuum mechanics, but informed from interatomic potentials. Here, we present and analyze our atomistic simulation results of homogeneous dislocation nucleation under Al(111) nanoindentation, in connection with the subsequently evolving embryonic dislocation loops. Focus will be on the comparisons of our simulation results with the above \( K \) criterion.
Fig. 6 shows the sequence of instantaneous defect evolution from the homogeneous nucleation of dislocation into the formation of dislocation embryos. As mentioned before, this type of initial defect structure, i.e., the Shockley partial dislocation loop embryonically bounding stacking-fault zone, has commonly been observed in the atomistic simulations of fcc(111) nanoindentations in the literature. Among close-packed {111} slip planes, (111) and (111) are the planes on which the two faces of embryonic dislocation loops are respectively grown in the current nanoindentation simulation. Fig. 6 also demonstrates that the two nucleation sites observed are located off the indenting axis below the contact surface. Approximately, its distance off the axis is measured to be $0.60a$ and the depth from the contact surface $0.50a$. Here $a$ denotes the nominal contact radius defined as $a = \sqrt{Rh}$ where $R$ is the indenter radius and $h$ the critical penetration depth. Our result is in good agreement with the nucleation depth of $0.51a$ that has been reported in the MD simulation of Al(111) nanoindentation by Van Vliet et al. (2003) (c.f., the off-axis distance is not available in their paper).

Applying the $K_c$ criterion for Cu(111) nanoindentation, Zhu et al. (2004) predicted the radial distance of $0.61a$ from the indenting axis and the depth of $0.58a$ from the contact surface. They identified that those nucleation sites correspond exactly to the three vertices of a regular triangle consisting of {111}-type slip planes. Furthermore, successively performed MD simulation of the same example confirmed their prediction. However, we found that the nucleation sites observed in our simulations were obviously different from those by Zhu et al. (2004). Before discussing this discrepancy, we first explain our results as follows. Fig. 7(a) illustrates two consecutive snapshots of dislocation nucleations obtained from our simulation. The two nucleation sites are well indicated by the defect-related atoms in red color, from which the embryonic dislocation loops develop promptly.\footnote{For interpretation of color in figure, the reader is referred to the web version of this article.}

The atoms in background are top-surface atoms. For the distinctive visualization of defects from those surface atoms in background, new color set is assigned to each value of centrosymmetry parameters in this figure only. Both snapshots are bottom views, and the indenting direction is thus outward normal to the paper. Now, let us draw two triangles denoted by A and B respectively in Fig. 7. Edges of both regular triangles are all on the {111}-type slip planes associated with the (111) indenting surface. The indenting axis goes through the center of these two concentric regular triangles.

According to their $K_c$ criterion, Zhu et al. (2004) stated that the dislocations are almost simultaneously nucleated at two of the three vertices ($A_1,A_2,A_3$) of the inner triangle, as mentioned earlier. Those three sites are equivalently favored for the homogeneous nucleation of dislocation. On
the other hand, our simulation reveals that the two embryonic dislocations grow respectively from two of the three equivalent middle points (B₁, B₂, B₃) on the edges of outer triangle, as can be seen from Fig. 7(a). It is of note that the three vertices of inner triangle (A₁, A₂, A₃) and the three middle points on the edges of outer one (B₁, B₂, B₃) are almost equidistant (~0.6a) from the indenting axis, as diagramed by the dashed circle in Fig. 7(b).

We further simulated the same model by changing the indenting conditions, one by one, such as the tip radius, the time step, the indenting speed, the first contact point, and so on. However, all simulations yielded the identical nucleation sites of the dislocation embryos, i.e., the middle points on the edges of outer triangle B. Note that the Λ criterion is parameter-free once the crystal lattice structure, such as fcc(111), and the interatomic potential are specified for the nanoindentation simulation. Zhu et al. (2004) used the Mishin potential (Mishin et al., 2001) for the demonstration of Λ criterion in Cu(111) nanoindentation, while we did the Ercolessi and Adams glue potential (Ercolessi and Adams, 1994) for our MD simulation of Al(111) nanoindentation. The different results between our simulation and the Λ criterion by Zhu et al. (2004), is therefore believed to be caused by the different interatomic potentials together with different materials indented.

To examine effects of the interatomic potentials employed, we performed the same MD simulations of both Al(111) and Cu(111) nanoindentations using another EAM potential proposed by Cai and Ye (1996). Both simulation results confirmed the homogeneous nucleation at the vertices of inner triangle A as in the case of Λ criterion. Furthermore, we also investigated the nucleation sites under Al(111) indentation through the molecular mechanics (MM) simulation with the Ercolessi and Adams glue potential and the conjugate gradient method. The model size is 17.7 (nm) × 17.8 (nm) × 10.5 (nm) of 208,008 atoms, and the bottom surface is fixed. All other conditions are the same as in the larger MD model. Since the MM simulation is an energy-minimization approach, it is impossible to precisely observe the transition state, i.e., the very exact instant of homogeneous dislocation nucleation. Therefore, we specified the nucleation sites indirectly. From the grown shapes of dislocation embryos, we could draw the overlapping triangle at the depth of 0.50a, and found that the triangle coincides with the outer one B of Fig. 7. It is accordingly inferred that the initial dislocations are nucleated at the middle of edges (B₁, B₂, B₃) as in our MD simulation of the same example with the same Ercolessi and Adams glue potential.

All the results from our simulations and other references available are summarized in Table 1 where the strong dependence of nucleation sites upon the interatomic potential chosen, not upon the materials indented, are well demonstrated. Therefore, from our experience up to this point, we expect that the Λ criterion for Al(111) nanoindentation might also result in the nucleation sites on the edges of outer triangle B as long as the
Ercolessi and Adams glue potential are used for assessing the criterion. If this is the case, those three spots \((B_1, B_2, B_3)\) could also be candidates for the nucleation sites of dislocations, each of which is equivalently favored for the homogeneous nucleation. Once the dislocations are nucleated at two of those sites, the embryonic dislocation loops are immediately developed along the two faces of the corresponding regular triangle \((B)\), as illustrated in Fig. 7. Comprehensive study of the homogeneous nucleation of dislocation under nanoindentation is expected to be further explored in the near future, focusing on the selection of specific interatomic potentials as well as other simulation conditions such as the indenter hardness.

### 4.2. Tetrahedral sessile lock

In spite of continued indenting load, the whole shape of aforementioned dislocation embryos remains nearly unchanged for some time until they suddenly transform into a tetrahedron at the second load relaxation \((\beta)\) in Fig. 2. The tetrahedron from molecular dynamics simulation has been shown in Fig. 3(b). This transition of defect shape followed by the load relaxation was also observed well in our molecular mechanics simulation of the same \(\text{Al(111)}\) nanoindentation, as shown in Fig. 8. The tetrahedron is constituted of four faces corresponding to \{111\} slip planes including the \{111\} contact surface, as illustrated in Fig. 9(b) and (c). Each face of the tetrahedron is the stacking-fault zone intersecting along the edges of \{110\} stairrod dislocations. Furthermore, Fig. 9(d) shows the cross sectional view of its empty interior, which implies that its inside is the region of perfect fcc single crystal. Therefore the tetrahedron is basically in the same form of stacking-fault tetrahedron, one of the common vacancy-type defect clusters in fcc metals of low stacking-fault energy.

A similar tetrahedral lock was also observed by Gannepalli and Mallapragada (2002) in their nanoindentation simulation of \(\text{Au(001)}\) with the indenter tip of pyramidal shape. However, the formation process of their tetrahedron was initiated from the edge of the contact region, which is completely different from the transitional formation of our current tetrahedral lock in \(\text{Al(111)}\) nanoindentation.

The current tetrahedron is gradually reconfigured into the irregularly shaped cluster of dislocation loops and stacking faults. During the relatively long period of (iii) in Fig. 2, observed are active appearing-and-disappearing motions of local dislocation loops along the \{111\}-type slip planes underneath the indenter tip. These multifaceted local glides of dislocations result in the highly oscillatory, but increasing overall, response in the load–displacement curve. From the moment of \((\gamma)\) in Fig. 2, one of the local dislocation loops finally grows to form the complete shape of prismatic partial dislocation loop accompanying the slow load relaxation during the step (iv). Its growth is portrayed in Fig. 4. The emission and glide of the fully developed prismatic partial dislocation loop will be dealt with in the following subsection.

### 4.3. Glide of prismatic dislocation loop

Long glides of partial dislocation loops have often been found when simulating nanoindentation.
tions of fcc crystals. In atomistic simulation of fcc(001) nanoindentation, Rodriguez de la Fuente et al. (2002) showed that dissociated dislocation loops consisting of two stacking-fault ribbons bounded by Shockley partial and a stair-rod dislocation were emitted and glided along the contact surface. From the MD simulations of nanoindentation on Al(111) surface, Li et al. (2002) and Van Vliet et al. (2003) observed that two parallel sets of dislocation segments, each having two partial dislocations separated by a stacking fault, were produced by several cross-slip events, and were in
downward motion along its glide prism, mediating further load relaxation. Those glides, either along the surface or through the thickness, are of great importance because they propagate the permanent (plastic) deformation far away from the vicinity of indenter tip.

In our MD simulation, the developed prismatic partial dislocation loop is completely separated from the local defect zone under the tip, around the instant of $(\delta)$ in the load–displacement curve of Fig. 2. The loop then begins its easy glide along $[0\bar{1}1]$ direction downward to the bottom surface as already shown in Fig. 5. Each of the four faces consists of a stacking-fault ribbon bounded by the edges of two Shockley partial and two stair-rod dislocations, being consistent with those in the literature. Two opposite pairs out of those four stacking faults are on $(\bar{1}1\bar{1})$ and $(1\bar{1}1)$ slip planes in this case as given in Fig. 10. According to Kelchner et al. (1998), the four faces can easily be identified to be stacking faults. In Fig. 10(c), shown is the two-layer-thick cross section of $(1\bar{1}1)$ plane on which one of the four stacking-fault ribbons lies. By out-of-plane pairing of atoms, we draw a vector (a small arrow) for each pair as illustrated in the figure. It exhibits that the directions of vectors inside the ribbon are slightly unparallel with those outside the ribbon, which implies clearly that the ribbon is the stacking-fault region bounded by partial dislocation loops. In Fig. 10(c), the four arrows in the lower right part stand for the perfect fcc configuration, while those in the upper left part indicate the atomic configurations after the loop passed by. The difference between those unparallel vectors thus corresponds the current partial Burgers vector (Kelchner et al., 1998).

Since we impose the free boundary condition on the bottom surface, this prismatic dislocation loop finally disappears to leave a parallelogram step on the bottom instead of bouncing back. Fig. 5(d) shows that all the edges of the parallelograms marked on the bottom surface are obviously parallel with the $\{111\}$ slip planes. Upon further indenting, similar prismatic partial dislocation loops are consecutively emitted from the contact

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**Fig. 10.** Glide of a prismatic Shockley partial dislocation loop: (a) the glide direction, (b) the structure of the dislocation loop, and (c) the two-loop thick cross section of $(1\bar{1}1)$ plane indicating the stacking-fault region. See the text for details.
region toward the bottom. Those downward glides of partial dislocation loops occur along either one among the three slip directions that are parallel with the three edges of the tetrahedron depicted in Fig. 9(c). That is, the loops induced by fcc(111) nanoindentation basically have no directional preference to follow among the three downward slip directions, the projections of which into the (111) plane have a three-fold rotational symmetry of 120°.

5. Concluding remarks

In this paper, we simulated Al(111) nanoindentations using molecular dynamics and molecular mechanics with particular emphasis on investigating the mechanism of incipient plasticity. An overall procedure of plastic deformation taking place inside Al single crystal was identified stepwisely according to changing phases of defect shapes. Of the whole procedure in defect evolution, some notable stages were analyzed in detail, focusing on the defect nucleation, dislocation locks, and specific evolution patterns while indenting Al(111) surface.

Using visualization of centrosymmetry parameters, we observed typical defects frequently found under nanoindentation of fcc single crystals, such as embryonic dislocation loops, a tetrahedral lock, prismatic partial loops. Structures and movements of those dislocation loops with stacking-fault zones can be well explained with the context of dislocation theories. We put our special attention on the homogeneous nucleation of dislocation under the tip. We confirmed that the nucleation sites of the initial dislocation loops are displaced from the indenting axis below the contact surface, consistent with the results already reported elsewhere. However, the exact locations of dislocation nucleation are different from some of the results predicted and simulated in the reference. Zhu et al. (2004) reported that the dislocations nucleated exactly at the vertices of right triangle associated with the fcc(111) slip system. On the other hand, we found that the sites were the middle points on the three edges of the triangle. We furthermore verified this discrepancy of nucleation sites came from the difference of interatomic potentials employed for simulation. More comprehensive atomic-level studies of homogeneous dislocation nucleations are thus expected in the near future, in relation with the shape and hardness of the indenter, for example.

As a present limitation of molecular dynamics simulations, unphysical wave reflection from the boundaries, especially from the bottom, of simulation domain may have chance to affect the triggering instants of dislocation generation and defect shape changes that are fundamentally instability phenomena at the atomic scale, as pointed out by many researchers as Liu et al. (2004a). In this paper, we therefore employed the free boundary for the bottom in order to minimize the unintended deterioration of defect mechanism due to wave reflection from the bottom surface. Quantitative studies of the effect of reflecting waves are believed to be proceeded along with the development of non-reflecting boundary condition for fully three dimensional molecular dynamics simulations. Temperature effect on the defect generation is another important aspect to be considered for realistic simulations of nanoindentation, which are under our investigation for the better understanding of incipient plasticity in fcc single crystals.

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