Computational Materials Science 115 (2016) 214–226

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Atomistic simulations of the nanoindentation-induced incipient plasticity in Ni_3Al crystal

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ARTICLE INFO

Article history:
Received 4 August 2015
Received in revised form 23 December 2015
Accepted 24 December 2015
Available online 2 February 2016

Keywords:
Nanoindentation
Dislocations
Atomistic modeling
Nickel based superalloys

ABSTRACT

In this work, the indentation-induced incipient plasticity of Ni_3Al crystal is investigated by performing molecular dynamics (MD) simulations. Simulation results reveal that the incipient plasticity of Ni_3Al is originated from the homogeneous nucleation of the $1/6\langle 1\,1\,2\rangle$-type Shockley partial dislocation. The critical load, critical contact pressure, dislocation nucleation site and active slip system are significantly affected by crystallographic orientation, model size, indenter radius and temperature. The choice of interatomic potential has significant implications for the indentation behavior of Ni_3Al. Some benchmarks for evaluating the credibility of interatomic potentials are presented. The pop-in phenomena are correlated with dislocation generation, multiplication and reactions. The formation mechanisms of complex stacking faults (CSFs), antiphase boundaries (APBs) and superlattice intrinsic stacking faults (SISFs) are clarified. The highest indentation modulus is obtained in (1 1 1) indentation followed by the (1 1 0) and (1 0 0) cases. The indentation modulus and the depth of nucleation sites increase with increasing indenter radius but the maximum shear stress decreases. The maximum shear stress and indentation modulus decrease linearly with increasing temperature, reflecting the stress-assisted and thermally activated nature of dislocation nucleation.

1. Introduction

Nickel-base superalloys are widely used in the hottest part of gas turbines for aircraft engines and power generation due to their superior high-temperature properties. Ni-base alloys exhibit a two-phase microstructure consisting of a face-centered cubic (FCC) Ni matrix (γ phase), strengthened by Ni_3Al precipitates (γ' phase). The Ni_3Al displays $L1_2$ ordered crystal structure with Al atoms at the cube corners and Ni atoms at the centers of the six faces of the cube. Since the mechanical properties of Ni-base alloys are derived from the properties of γ' phase, a great deal of research work has been done on the deformation mechanisms of Ni_3Al crystal [1].

To investigate the ultimate strength and incipient plasticity of Ni_3Al crystal, a number of nanoindentation experiments have been performed for γ' phase [2–10]. For example, the nanoindentation of Ni_3Al has been performed for the (1 1 1), (1 1 0) and (1 0 0) crystal surfaces [5,6]. The indentation behavior of Ni_3Al is found to be closely related to crystallographic orientation, pre-existing dislocation density, temperature as well as indenter radius [5–7]. During a typical nanoindentation test, a stiff indenter penetrates into a surface, while the contact load is recorded as a function of displacement. The load–displacement (P–h) curves frequently show a characteristic set of discontinuities, or called as pop-in events, e.g. sudden depth excursions under load control [2,3] or sudden load drops under displacement control [11]. The occurrence of the first pop-in is widely believed to be indicated the onset of plasticity and associated with homogeneous nucleation of dislocation loop since the maximum shear stress under the indenter can approach the theoretical shear strength of materials [12–19].

The pop-in phenomena in nanoindentation provide insights into the origins of dislocation nucleation in initially defect-free crystals. Although the dislocation configuration in Ni_3Al was examined by the transmission electron microscopy (TEM) [3,4], it is still unclear how the initial dislocations multiply during the early stages of plastic deformation due to the limitations of conventional TEM technology. For example, the mechanical cutting and lapping processes for preparing TEM specimens will damage the dislocation patterns. Furthermore, the TEM observation is only available post-mortem and unable to capture the ongoing mechanisms of plasticity. The recent development of in situ nanoindentation techniques have enabled the real-time observation of the dislocation generation during indentation processes [13]. However, the typical

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http://dx.doi.org/10.1016/j.commatsci.2015.12.045
0927-0256/

video sampling rate is about 30 frames per second, which is too slow to capture the movement of individual dislocations [20].

As an essential and helpful complement to experiments, atomistic simulation provides a real-time monitoring of the deformation mechanism of crystals during indentation process, such as dislocation nucleation, motion and reactions. Atomistic simulations have been extensively applied to investigate the indentation behavior and incipient plasticity for many materials, particularly for face-centered cubic (FCC) [21–24] and body-centered cubic (BCC) [25–28] crystals.

In this paper, the incipient plasticity in Ni_3Al nanoindentation was investigated by performing large-scale molecular dynamics simulation for Ni_3Al (100), (110) and (111) crystal surfaces. The effects of crystallographic orientations, interatomic potentials, model sizes, indenter radii and temperatures on the incipient plasticity of Ni_3Al were studied systematically. The correlation between dislocation generation and pop-in events during nanoindentation process was analyzed in detail.

2. Method

Choosing an appropriate interatomic potential is crucial for atomic simulations. The embedded atom method (EAM) potentials are extensively used in atomistic simulation for metallic systems, due to their accuracy and computational efficiency [29,30]. For Ni–Al binary system, several EAM potentials have been constructed by fitting to experimental data and first-principles results [31–35]. In this work, four widely used EAM potentials were selected to descript the interatomic interaction in Ni_3Al and denoted by year of publication, i.e. the EAM89 was developed by Chen et al. in 1989 [31]; the EAM04 [32] and EAM09 [33] were developed by Mishin et al. in 2004 and 2009, respectively; the EAM13 was developed by Du et al. in 2013 [34]. These EAM potentials can reasonably reproduce many physical properties of γ' phase in Ni-based superalloys.

In this work, the Ni_3Al nanoindentation was simulated by classic molecular dynamics to investigate the underlying mechanism of incipient plasticity in Ni_3Al crystal. An initially defect-free Ni_3Al single crystal with size of $20\,nm \times 20\,nm \times 20\,nm$ was constructed as an indented substrate, without considering the impact of pre-existing defect. In experiment, the smallest tip radius was down to the region of 30–100 Å [12,36]. Given this, a rigid spherical indenter with radius (R) of 50 Å was penetrated into three low-index crystal surfaces of Ni_3Al, i.e. (100), (110) and (111). The base vectors **x**, **y** and **z** were set as [001], [100], [010] for the (100) indentation; $[1\bar{1}0]$, [110], [001] for the (110) case; $[11\bar{2}]$, [111], $[1\bar{1}0]$ for the (111) case. The contact surface was free, while other boundaries were fixed to avoid rigid body motion during indentation. The indenter was modeled as a repulsive force: $F(r) = -K(r-R)^2$ for $r < R$, and $F(r) = 0$ for $r \geqslant R$, where r is the distance from an atom to the center axis of indenter, R is the indenter radius, $K = 10\ eV/Å^3$ is the stiffness coefficient.

To reduce the effect of thermal fluctuation on dislocation processes, the atomistic simulations of nanoindentation were carried out by LAMMPS [37] at low temperature 1.0 K and controlled by Nose–Hoover thermostat [38]. MD simulation at such low temperatures does not allow atomic reorganization and these simulations would seem to me to be closer to geometry optimizations, thus, the temperature effects can be neglected at the extremely low temperature in the MD simulations. The initial relaxation was performed properly for 100 ps before indentation. The indenter was allowed to move toward the contact surface with a speed of 1 m/s. The time step of simulation was set as 1.0 fs. Note that the applied loading rate is higher than that in experiments. This excessively large speed originates from the intrinsic limitation of atomistic simulation on time scale [23,39].

The analysis of centrosymmetry parameter (*CSP*) was performed to selectively visualize the interior defects induced by nanoindentation. The *CSP* is defined as [21]

$$CSP = \sum_{i=1}^{N/2} \left| \mathbf{R}_i + \mathbf{R}_{i+N/2} \right|,$$

where N is the nearest neighbors of atom, $\mathbf{R}_i$ and $\mathbf{R}_{i+N/2}$ are the vectors from the central atom to a particular pair of nearest neighbors. According to this definition, the *CSP* is zero for an atom that locates at the site of perfect lattice and non-zero for an atom that is near a defect. With the help of *CSP*, the indentation-induced defects, i.e. vacancies, dislocations and stacking faults (SFs), can be visualized using a free software AtomEye [40]. The Burgers vector of dislocation was calculated using a modified Nye-tensor method [41–43]. The implementation of the modified Nye-tensor method can be found in the work of Begau et al. [41,42].

3. Results

The main outcome of a depth-sensing indentation test is the load–displacement (P–h) curve. Fig. 1 plots the P–h curves of Ni_3Al for four EAM potentials. Initially, the Ni_3Al substrate undergoes a nonlinear elastic deformation. The contact load (P) increases monotonically with increasing indentation depth (h). At the elastic stage, there are no defects inside the substrate. When P increases to a critical value, a sudden load drop occurs in P–h curves, called as the first pop-in event. Extensive experiments demonstrate that the first pop-in event is associated with the nucleation or activation of dislocations [12–19].

As shown in Fig. 1, Ni_3Al crystal exhibits strong anisotropic characteristics in nanoindentation. The number of pop-ins and the critical load for the first pop-in event are dependent on surface orientations and interatomic potentials. For all of four potentials, the critical load required for the first load drop in (111) indentations is larger than that in (110) indentations (Table 1). The magnitude of the first load drop in (111) and (110) indentations is larger than that in (100) indentation, especially in the EAM09 case (Fig. 1c), no obvious load drop was observed in whole process ($h < 10$ Å).

As mentioned previously, the first pop-in event observed in nanoindentation is usually regarded as an indicator of dislocation nucleation. However, in the Ni_3Al nanoindentation, the first pop-in is not an accurate indicator of incipient plasticity since the dislocation nucleation event occurs before the first load drop in (100) nanoindentations (Fig. 1b and c). Similar behavior was observed in the nanoindentation of Co crystal [44]. The first pop-in should not be regarded as a criterion for judging crystal instability [44]. More accurate instability criterion is needed for predicting the indentation-induced crystal instability [45–47]. The critical indentation depth (h_c) and critical contact load (P_c) required for dislocation nucleation in Ni_3Al nanoindentations are listed in Table 1. It is seen that the values of P_c in the (100) indentations are smaller than those in the (110) and (111) cases.

Another anisotropic character is reflected in the stiffness of crystal surfaces. From the P–h curves in Fig. 1, it is clear that the (111) surface is more rigid than the (110) and (100) surfaces. The stiffness of the indented surfaces is characterized by indentation modulus (E^*). As a frictionless contact problem, the contact load between an elastic half-space surface and a rigid sphere with radius of R can be described by the Hertzian model, $P = 4/3E^*R^{1/2}h^{3/2}$ [48]. The values of E^* can be extracted by fitting the P–h curve prior to the onset of plasticity using the Hertzian model. The dash-dot–dot lines in Fig. 1a illustrate the elastic deformation following