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Atomistic modeling for mechanism of crack cleavage extension on nano-scale

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ABSTRACT

The crack cleavage extension on nanoscale within the triangular lattice of a fcc materials is addressed. The crack propagation behavior of the sample without and with different pre-straining level under tensile strain is simulated using the advanced phase field crystal (PFC) method. It can be founded that for samples with pre-straining along $[\bar{1}\ 1\ 0]$ of X direction, the crack propagation characteristics of the extending-turning–extending are presented, which appears the zigzag edge of the crack; while for samples with pre-straining along $[\bar{1}\ \bar{1}\ 2]$ of Y direction, the crack propagation at the later stage presents longer cleavage crack extension along with the stress concentration of the dislocation at crack tip, which direction is about $[1\ \bar{2}\ 1]$ and $[\bar{1}\ 2\ \bar{1}]$. The PFC model combined with the diatomic spring model is used to reveal the mechanism of the cleavage crack start-up and extension on nano-scale.

1. Introduction

The level of pre-plastic strain introduced into material can significantly change mechanical properties and also effect on subsequent mechanical and fracture behavior of engineering alloy [1–4]. The influence of the plastic pre-strain on the deformation and creek initiation and growth behavior has been one of focus in engineering fracture mechanics studies in recent years [5,6]. For example, the 316H stainless steel with plastic pre-strain is of accelerated cracking behavior compared to its parent steel [7]. However, the initiation and growth of the microcrack are actually nanoscale problem. For this reason, engineering fracture mechanics is no longer suitable in nano-scale crack. Although there are many research reports on the crack propagation [8,9], it still lacks the research of deepening into the atomic level to reveal the mechanics of the crack propagation, which need to study the atomic dynamic surrounding the crack tip [10]. The breaking of the atomic bond at creak tip is a dynamic and highly nonlinear process, which cannot be explained under the continuum mechanics assumption [11]. Although phenomenological continuum theories are sophisticated in most engineering applications, due to the atomic nature of fracture, e.g. bond-breaking, in some case the continuum framework fail to correctly predict the nature of the crack dynamic in materials [10]. There are some of the reasons that make the use of atomic level simulations essential [11–13]. Many research have used the atomistic level simulation model of the crack and fracture, including molecular dynamics (MD) simulation [10]. Even though the standard molecular dynamics (MD) simulation [13] provides detailed information about atomistic processes, they generally limited to time scales [14,15] of picoseconds (10^{-12} s) and relatively small sample (10^7 atoms) which lead to more high stresses (GPa) and strain rates [14] ($10^7\ s^{-1}$) to be contrasted with much slower experimental strain rates of $10^{-5}\ s^{-1}$ to $10^{-3}\ s^{-1}$ [15].

Recently, Elder et al. [16] proposed a new atomistic method, i.e. phase field crystal (PFC) model with an advantage on diffusive time (10^{-6} s) scales for simulating microstructure evolution. This method naturally incorporates elastic and plastic deformations and multiple crystal orientations and can be used to study many important material processing phenomena [17–19], including crack growth and branch on nano-scale [20,21]. The PFC method is not aimed at a specific material and is able to describe crystallographic structure and captures the nonlinear elastic behavior of the crystal, therefore, the model is more suitable for revealing the details of the dislocation movement and of the crack initiation and growth at nano-scale [16,20]. There are many experimental reports [5–7] of the crack initiation and propagation under the pre-straining level, however, the mechanism research of the simulation experiment of the crack with different pre-straining level at nano-scale is no reported so far as we know. The purpose of this paper is that on the basis of the modified PFC model [20,22], we study the system with different pre-straining level and simulate

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the evolution process of the nano-crack initiation and propagation under uniaxial tension, analyze the effects of the different pre-straining level on the crack initiation and propagation with dislocation, and reveal the mechanism of the nano-creak cleavage and of the blunting by the modified PFC combined with the diatomic spring model [12].

2. Model and method

2.1. Modified PFC model and kinetic equation

Based on the classical density functional theory (CDFT), we can deduce the simple dimensionless free energy functional model with direct correlation function type proposed by Elder et al. as below

$$\widetilde{F} = \int d\vec{x}\left\{\frac{\rho(\vec{x})}{2}[(e+1)\rho(\vec{x}) - K_{Elder}] + t^*\frac{\rho(x)^3}{3} + \frac{\rho(\vec{x})^4}{4}\right\}, \tag{1}$$

where $K(\vec{r})_{Elder} = C_2(\vec{x})\rho = [1-(\nabla^2+1)^2]\rho$, ∇^2 is the Laplace operator, e and t^* are constants, and relate to temperature and the anisotropy of interface, respectively; ρ is the rescaled time-averaged atom number density measured with respect to a reference liquid state [22].

Here we do not discuss solid-liquid interface anisotropy, therefore, t^* can be ignored it and set $t^* = 0$, then the formula (1) can be written as:

$$\widetilde{F} = \int dV\left\{\frac{\rho(\vec{x})}{2}[e+(\nabla^2+1)^2]\rho(\vec{x}) + \frac{\rho(\vec{x})^4}{4}\right\} \tag{2}$$

Therefore, the free energy functional of the system with the density function ρ measured with a reference liquid state ρ_0 is obtained, i.e., the original PFC [16] suggested by Elder. The direct correlation function operator $C_2(\vec{x})$ can be written as $C_2(\vec{x}) = [1-(\nabla^2+1)^2]$ from Eq. (2). Jaatinnen et al. [23] demonstrated that the parameter e can be identified as $e \propto \frac{1}{S(k_m)}$, $S(K_m)$ is the structure factor, K_m is the first peak position.

It can be obtained an analytical expression for Eq. (2) in the one-mode approximation [16] under the minimum of the free energy. Then, the atomic density for two-dimensional triangular structure can be written as

$$\rho = \rho_1 - \rho_0 = A_T[\cos(qx)\cos(qy/\sqrt{3}) - \cos(2qy/\sqrt{3})/2] \tag{3}$$

where

$$\rho_1 = A_T[\cos(qx)\cos(qy/\sqrt{3}) - \cos(2qy/\sqrt{3})/2] + \rho_0, \tag{3'}$$

where ρ_0 is the average density value as a reference, the wave vector $q = \sqrt{3}/2$, $A_T = \frac{4}{15}(3\rho_0 - \sqrt{-36\rho_0^2 - 15r})$.

We assume that the inter-atomic potentials of all particles in a crystal are bonded between any paired-particles. The interatomic potential of the nearest neighbor of the PFC model can be approximately deduced from formula (2) by following Ref. [16] as

$$\mathrm{H}(r) = \mathrm{V}_0\left[-2\left(\frac{a_0}{\mathrm{r}}\right)^2 + \left(\frac{a_0}{\mathrm{r}}\right)^4\right]. \tag{4}$$

where r is the distance of the nearest atoms and the V_0 is the bond energy, and a_0 is the reference inter-atomic distance without external load.

Under the external applied strain ε on the system with tensile along $[\bar{1}\ \bar{1}\ 2]$ direction for deformation, we can write the energy of system as

$$\widetilde{F} = \int f(\rho(x, y(1+\varepsilon)))dV = \int [f(\rho(x,y)) + E_{ext}(\varepsilon, x, y)]dV, \tag{5}$$

where $E_{ext}(\varepsilon, x, y)$ is the energy change of system due to the strain. According to Refs. [20,24], the form of the energy density change can be selected as $E_{ext} = V_{ext}\cdot\rho$, where V_{ext} is the external force field. The benefits of this approach is that the modified free energy in Eq. (5) has the same phase diagram as that in Eq. (2). The more details for V_{ext} will be given in the next section.

Then the Cahn-Hilliard evolution equation of the dimensionless of the atomic density is described by [16,20] as below

$$\frac{\partial\rho}{\partial t} = \nabla^2\frac{\delta\widehat{F}}{\delta\rho} = \nabla^2[e\rho + \rho^3 + (1+\nabla^2)^2\rho + V_{ext}], \tag{6}$$

Then the evolution of the atomic density is described by the nonlinear six order differential equation (6), the numerical discretization of which is implemented using the semi-implicit Fourier spectral method [22–28].

2.2. Simulation sample preparation

For the sake of simplicity, the simulation experiments are performed in two-dimensional (2D) triangular lattices [10] which represent the close-packed planes of FCC shown in Fig. 1. What we choose the 2D lattice for the simulation experiment is based on the Ref. [28]. In present work, we chose a single crystal sample with a orientation angle $\theta = 3.5°$ by $[\bar{1}\ 1\ 0]$ direction of x axis as shown in Fig. 2(a) and a notch at the center of the sample as an initial nano-crack in Fig. 2(b). The parameters for the single crystal sample and for the notch are shown in Table 1.

Although the PFC method does not directly model a solid-vacuum interface [27] as the MD simulation [27] to deal with the crack region, according to the Refs. [20,29] of the soft phase to describe the crack pattern, we can use the solid phase region transforming into liquid phase region to show the pattern of the crack growth and extension. A similar approach are given in Refs. [16,20,28–30]. We implement the simulation on two-dimensional (2D) sample with 1024×512 grid points (gp), about $64 * 36\ \mathrm{nm}^2$, where the grid size is $\Delta x = \Delta y = \pi/3$ and time step $\Delta t = 0.05$. The periodic boundary conditions are applied in all four edges. A notch with a 14×14 gp is set in the center of the sample as an initial crack. The method for setting pre-straining of the sample: Modifying the atomic density function (3) of the triangular phase, we get the density function with pre-straining are $\rho(x(1+\eta_x), y)$ and $\rho(x, y(1+\eta_y))$, where η_x and η_y represents the dimensionless pre-straining along x and y direction. The samples with different pre-straining level are shown in Table 1, in which the ρ_K is the density for the notch shown in PFC phase diargram in Ref. [20].

2.3. Applied strain and the displacement field

Following the Ref. [20], the detail form of the force field V_{ext} is set as

$$\begin{aligned} V_{ext} &= V_y(\varepsilon) \\ &= A\left[\cos(qx)\cos(qy(1-\varepsilon_y)/\sqrt{3}) - \frac{1}{2}\cos(2qy(1-\varepsilon_y)/\sqrt{3}))\right] \\ &= \rho_y(y), \end{aligned} \tag{7}$$

Here we set $\varepsilon_y = \varepsilon$, and A is a constant and is set as 1. To do the deformation with it, it is needed usually to design a modulation function [31] to be used to describe the boundary shape. To do so, its implementation is rather complicated and tedious. While the applying strain method in PFC model under constant volume