Physica B: Condensed Matter 552 (2019) 104–109

Contents lists available at ScienceDirect

Physica B: Condensed Matter

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

The influences of crystal orientation and crack interaction on the initiation of growth and propagation mode of microcrack: A phase-field-crystal study

Shi Hu[a,*], Song Wang[b]

[a] College of Civil Aviation Safety Engineering, Civil Aviation Flight University of China, Guanghan 618307, China
[b] School of Materials Science and Engineering, Northwestern Polytechnical University, Xi'an 710072, China

ARTICLE INFO

Keywords:
Crack growth
Crack propagation
Crystal orientation
Crack interaction
Microcrack
Phase-field-crystal

ABSTRACT

Phase-field-crystal (PFC) method is applied to study the influences of crystal orientation and crack interaction on the initiation of growth and propagation mode of microcrack under uniaxial strain in nanocrystal system. The microscopic mechanism is explored through mono- and dual-crack systems. Results show that the crystal orientation and crack interaction have no influences on the initiation of growth of microcrack, all simulation systems have an identical critical strain of crack growth. On the other hand, the two influential factors can observably alter the propagation mode of microcrack. With the increase of crystal orientation, crack propagation mode changes from cleavage mode to a mixed-mode of ductile fracture and cleavage. The influences of crack interaction on the propagation mode of microcrack are various. If crack tips move in the same direction, crack propagation mode can be changed. On the other hand, if crack tips move toward each other, crack propagation mode will not be varied, but the specific interaction results are different depending on the value of crystal orientation. Through this research, the PFC simulation is demonstrated to be an effective means to study multiple microcrack propagation behavior.

1. Introduction

Microcracks can hardly been avoid in strained metals [1,2]. Under certain conditions, these microcracks will start to propagate. Among various influential factors, crystal orientation [3,4] and crack interaction [5–7] have been proved to have significant impact on crack evolution behavior. Meanwhile, the initiation of growth and propagation mode of microcrack, which determine the service life of engineering materials to some extent, are actually nanoscale problems. Therefore, it is hard to directly and continuously track microcrack evolution by traditional experimental methods.

Computational materials science [8,9], which is a cross-discipline of mathematics, physics, computer science and materials science, has developed rapidly in the early twenty-first century. It presents a new approach to research the nanoscale evolution mechanism of microcrack. Based on density functional theory [10], Elder et al. [11] propounded phase-field-crystal (PFC) method. The PFC method can simulate transformation of atomic scale structure [12,13] and evolution of materials on diffusion time scale [14,15], which makes it particularly suitable for studying microstructure evolution in crystals [16–19]. Therefore, it is widely used to solve various materials problems [20–24], of which simulation results are in good agreement with theories and experiments. In addition, as many modified PFC methods have been proposed [25–28], the application range of PFC method is significantly extended.

In the research field of microcracks, much meaningful work has been achieved by using the PFC model. For example, Gao et al. [29–31] have thoroughly explored the crack propagation behavior in monocrystal system under different pre-strains. However, crystal orientation effect is not taken into consideration. In actual materials, as orientations of crystalline grains are randomly distributed, it is necessary to study the influence of crystal orientation on crack behavior. In addition, most PFC results of crack propagation are obtained from mono-crack samples [29,31–34]. Crack interaction, with the exception of crack connection [30], is seldom touched. Therefore, different results and mechanisms of crack interaction in dual-crack samples are also worth researching.

In this work, we use the PFC method to study the influences of crystal orientation and crack interaction on the initiation of growth and propagation mode of microcrack in nanoscale dual-crack system. The rest of this work is arranged as follows: In Sec. 2, the simulation methods used are introduced, including one-mode PFC method, dynamic equation, strain application and simulation system design. In Sec. 3, simulation results and discussion are provided. Lastly, important

* Corresponding author.
E-mail address: hshi@mail.ustc.edu.cn (S. Hu).

https://doi.org/10.1016/j.physb.2018.10.002
Received 26 August 2018; Received in revised form 29 September 2018; Accepted 1 October 2018

conclusions obtained in this work are given in Sec. 4.

2. Simulation methods and system construction

The simulated crystal structure represented by the triangular lattice is built on the one-mode PFC model put forward in Ref. [11]. The dimensionless free energy functional can be written as:

$$F = \int dx\{\frac{\varphi}{2}[r + (1 + \nabla^2)^2]\varphi + \frac{1}{4}\varphi^4\} \tag{1}$$

In this formula, $\phi(\boldsymbol{R})$ is the order parameter representing dimensionless crystal density field, of which ϕ is periodic local atomic density and $\boldsymbol{R}$ is space coordinate. The maxima of ϕ represent atomic positions in the solid phase. Specifically, the density field of liquid phase has a uniform value. r is dimensionless degree of subcooling that indicates the system temperature. ∇^2 symbolizes the Laplace operator.

The expression of ϕ can be written in a general form:

$$\varphi(\boldsymbol{R}) = \sum_{n,m} a_{n,m} e^{i\boldsymbol{G}\cdot\boldsymbol{R}} + \varphi_0 \tag{2}$$

where ϕ_0 is the average atomic density. $\sum a_{n,m} e^{iG\cdot R}$ reflects the periodic structure characteristics of lattice atoms. $G \equiv nb_1 + mb_2$, for triangular lattice, the reciprocal lattice vectors $\boldsymbol{b_1}$ and $\boldsymbol{b_2}$ can be written as:

$$\boldsymbol{b}_1 = \frac{4\pi}{a\sqrt{3}}(\frac{\sqrt{3}}{2}\boldsymbol{x} + \frac{1}{2}\boldsymbol{y}),\ \boldsymbol{b}_2 = \frac{4\pi}{a\sqrt{3}}\boldsymbol{y} \tag{3}$$

where a is the distance between nearest-neighbor local maxima of ϕ.

Using one-mode approximation, the atomic density of triangular lattice can be expanded as follows:

$$\varphi = \varphi_0 + A_t[\cos(q_t x)\cos(\frac{\sqrt{3}}{3}q_t y) - \frac{1}{2}\cos(\frac{2\sqrt{3}}{3}q_t y)] \tag{4}$$

where q_t is wave number, satisfying $q_t = 2\pi/a$, and A_t is density wave amplitude. The values of q_t and A_t can be obtained by substituting Eq. (4) into Eq. (1) and minimizing the resulting free energy with respect to q_t and A_t. Thus, q_t and A_t are acquired as:

$$q_t = \frac{\sqrt{3}}{2},\ A_t = -\frac{4}{15}(-3\varphi_0 - \sqrt{15r - 36\varphi_0^2}) \tag{5}$$

Meanwhile, this minimization yields the free energy of triangular lattice:

$$F_{tri} = \tfrac{13}{500}\varphi_0^4 + \tfrac{16}{125}\varphi_0^3\sqrt{15r - 36\varphi_0^2} + \tfrac{7}{50}r\varphi_0^2 - \tfrac{4}{75}\varphi_0 r\sqrt{15r - 36\varphi_0^2} + \tfrac{1}{10}r^2 - \tfrac{1}{2}\varphi_0^2 \tag{6}$$

By taking differentiation of free energy with respect to triangular and liquid phase density fields and using common tangent law, the two-dimensional phase diagram can be derived as shown in Fig. 1.

As atomic density field is a conserved value, the dynamics evolution of ϕ is solved by the MPFC model proposed by Stefanovic et al. [35], which is given by:

$$\frac{\partial^2\varphi}{\partial t^2} + \beta\frac{\partial\varphi}{\partial t} = \alpha^2\nabla^2\frac{\delta F}{\delta\varphi} \tag{7}$$

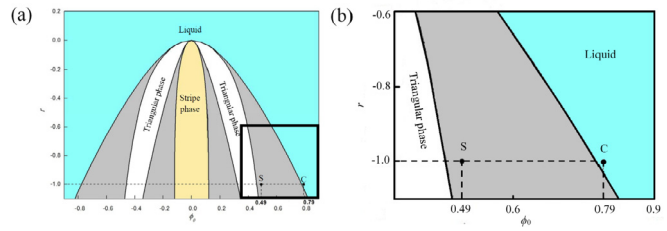

Fig. 1. Two-dimensional phase diagram calculated by the one-mode approximation (gray regions correspond to two-phase coexistence zones). Panel (b) is the enlarged image of the area enclosed by black solid box in panel (a).

where α and β are constants, related to effective sound speed and vacancy diffusion. α and β are adopted as 15 and 0.9, respectively.

In this work, uniaxial strain along y-direction is applied through traction boundary conditions, which are incorporated into Eq. (1) by using a new penalty term [36]. After equilibration of the constructed simulation systems, the uniaxial strain is applied at a slow constant strain rate of $\varepsilon' = 6 \times 10^{-6}/\Delta t$, of which Δt is time-step and equals 0.3, by displacing the penalty function. The details of penalty function, strain application and numerical algorithm of the nonlinear dynamic Eq. (7) can be found in Ref. [36], therefore will not be described here.

The entire simulation region is predetermined as a square scaled with $L_x \times L_y$ ($L_x = L_y = L$), and periodic boundary conditions are imposed in all directions. In order to create a triangular structure with crystal orientation θ, coordinate transformation of Eq. (4) is performed as follows:

$$\begin{cases} x = x'\sin\theta + y'\cos\theta \\ y = x'\cos\theta - y'\sin\theta \end{cases} \tag{8}$$

where (x', y') and (x, y) indicate coordinates before and after this conversion.

Using Eqs. (1), (4) and (8), we create triangular lattice structure with crystal orientation θ. System parameters are set up as follows: Grid-sizes are $\Delta x = \Delta y = \Delta L = \pi/4$ and side length of the square system is $L = 512\Delta L$. Average atomic density is $\phi_0 = 0.49$. Temperature parameter is chosen to be $r = -1.0$.

To explore the influences of crack interaction on the initiation of growth and propagation mode of microcrack, mono- and dual-crack systems both have to be constructed. Gaps in the central area of solid phase are precast as initial cracks. Each gap is a rectangle scaled by $50\Delta L \times 15\Delta L$. Atomic density of gap region is set to be $\phi_c = 0.79$, as point C shown in Fig. 1. Point C is close to the coexistence line (Fig. 1(b)), which benefits the transformation from triangular phase to crack structure and the propagation of microcrack [29,32,34]. For dual-crack system, distances between the two gap centers along x- and y-directions are D_x and D_y, respectively. D_y is set to be constantly equal to $58\Delta L$. The illustration of dual-crack system studied in this work is given in Fig. 2. We also give the schematic diagram of crystal orientations in Fig. 2. Table 1 shows the values of constant parameters used in this work.

3. Results and discussion

3.1. The influences of crystal orientation and crack interaction on the initiation of growth of microcrack

In this section, we explore the influences of crystal orientation and crack interaction on the initiation of growth of microcrack. Critical strain of crack growth is used to judge whether the initiation of growth is promoted or obstructed.

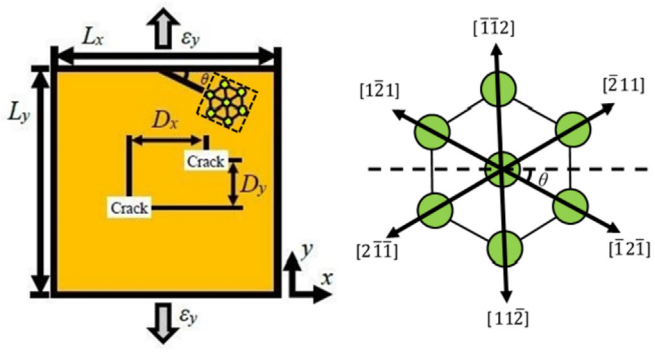

Fig. 2. Schematic diagram of dual-crack system and crystal orientations employed in this work. ε_y is strain applied along y-direction.