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Size effects of shear deformation response for nano-single crystals examined by the phase-field-crystal model

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ABSTRACT

Employing the modified phase-field-crystal (MPFC) model, we investigated the size effects of shear deformation response on nano-single crystals by examining the elastic strain distribution at atomistic scales. Here, three specimens with different aspect ratios are explored. Three types of shear deformation behavior have been found, namely, bending, simple shear and the mixed-mode based on the competition of bending and shearing. Further, a size scale analysis indicates that the slope of the shear strain response curve decreased dramatically as the aspect ratio changed from 1 to 0.125. However, when the ratio increased from 1 to 8, the slope increased slowly until saturated.

1. Introduction

The degree of materials strengthening in a wide range of metallic systems is highly dependent upon shapes, sizes and local variables of shearable precipitating nanoparticles (NPs). These NPs can always be found in various cases, such as second phase precipitates in aluminum alloys [1–4], shear deformations in metallic nanoparticles [5] and the laser pulse induced deformation of nanoparticles [6]. Among them, shear deformation response of NPs is an hot topic, and various models have been proposed to clarify the strain response of NPs [2]. However, quantitative relationship between the strain state and the shape or size of NPs in experiments is still absent, especially for some intrinsically strained or under external applied strain NPs. It is hard to characterize the strain state using standard experimental techniques, as the size of NPs is very small, usually ranged from few to a dozen nanometers. Therefore, it is necessary to develop new valid methods to quantitatively characterize these strained NPs.

With the development of computer science, modeling and simulation has been a powerful tool in studying microstructure evolution of materials. At present, molecular dynamics (MD) method is usually adopted to study deformation behaviors at atomic scales [7,8]. However, the standard MD method is limited to a very short time scale (Nano-second). This limitation is very severe in developing MD models to study the physical and mechanical behaviors of nanostructured materials, where the relevant length scales are atomic but the time scales are diffusional.

Progress toward alleviating this limitation has recently been made by introducing a new methodology known as the phase field crystal (PFC) model, which is an extension of the dynamical density functional theory [9–11]. The PFC model was developed by Elder et al. [9,12] and then subsequently applied to many situations such as polycrystalline solidification [13,14], phase transitions [15], fracture [16,17], elasticity [18], dislocation dynamics [19], and vacancy dynamics [20]. Because the PFC model automatically contains elasticity, the energy difference between the unstrained state and the strained one, Δf, can be expressed through a quadratic function, related to the elastic constants. For a detailed calculation of the elastic constants, the reader is referred to the work of Pisutha-Arnold et al. [21]. Unfortunately, the original PFC model evolves the mass density only at diffusive time scales, so it cannot adequately describe elastic responses in strained crystals. In order to overcome this drawback, Stefanovic et al. introduced a newly modified phase field crystal (MPFC) that includes both diffusive dynamics and elastic interactions [18,22,23].

In the present paper, in order to precisely characterize the strain state of NPs, we will restrict NPs to the simple case where the particle could be considered as a nano-single crystal. Then the MPFC model is employed to investigate the linear elasticity response process in the nano-single crystal specimens with different aspect ratios. We characterized the effects of length scales on the strain

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state of nano-single crystal quantitatively. This work can also prompt the MPFC method to quantitatively investigate atomic physical properties.

2. Model description and strain characterization

2.1. The MPFC model

In the PFC formalism, an order parameter φ defined as the local-time-averaged atomic number density is used to describe a material state. In contrast to conventional phase field (PF) models, the order parameter in PFC models is not a spatially constant, but exhibits periodic modulations in a crystalline phase corresponding to atomic positions. For simplicity, here we use the original dimensionless free energy functional F [9,12]

$$F = \int \left[\frac{r}{2}\varphi^2 + \frac{1}{4}\varphi^4 + \frac{\varphi}{2}(1+\nabla^2)^2\varphi\right] d\mathbf{r}, \tag{1}$$

where φ is the rescaled time-averaged atom number density measured with respect to a reference liquid state, and r is a control parameter, corresponding to a dimensionless temperature.

In the original PFC model, the dimensionless evolution kinetic equation for the order parameter φ is

$$\frac{\partial \varphi}{\partial t} = \nabla^2[r\varphi + \varphi^3 + (1+\nabla^2)^2\varphi], \tag{2}$$

The above kinetic equation propagates all disturbances (elastic and plastic) diffusively. This would restricts the scope of reproducible phenomena to those whose characteristic time is comparable to the diffusive time scale, such as phase transitions and slow mechanical transformations. And the kinetic equation also prevents PFC simulations from direct comparison with faster, real-world mechanical experiments. To handle this shortcoming of PFC, a modified PFC (MPFC) dynamic equation is introduced by Stefanovic et al. [18], which is given by

$$\frac{\partial^2 \varphi}{\partial t^2} + \beta\frac{\partial \varphi}{\partial t} = \alpha^2\nabla^2[r\varphi + \varphi^3 + (1+\nabla^2)^2\varphi], \tag{3}$$

where α and β are phenomenological constants related to the effective sound speed and vacancy diffusion coefficient respectively. Eq. (2) is of the form of a damped wave equation, containing two propagating density modes at the early stage and one diffusive mode at late times. By choosing effective values of α and β, a finite elastic interaction length and stage can be set. Over this elastic interaction time and distance, density waves will propagate effectively undamped. Beyond this time and distance, however, density evolution becomes diffusive. For more information one can refer to Ref. [18]

The thermodynamic phase diagram of this model has been discussed previously [9,12,24], which shows that the free energy functional of Eq. (2) can yield different crystal phases such as body-centered-crystal lattices, hexagonal lattices and the lamellar phase. In this study, we restrict our attention to hexagonal lattices in two dimensions. The hexagonal lattice density in two dimensions can be approximated by considering the contribution of the principle reciprocal lattice vectors as:

$$\begin{aligned}\varphi(\vec{r}) &= \varphi_0 + \sum_i A_i e^{i\vec{k}_i\cdot\vec{r}} \\ &= \varphi_0 + A[\cos(qx)\cos(qy/\sqrt{3}) - \cos(2qy/\sqrt{3})/2],\end{aligned} \tag{4}$$

where φ_0 is the average density, q is wave number related to the crystal lattice constant a_0 ($q = 2\pi/a_0$), and A is the amplitude of density waves. By substituting Eq. (4) into Eq. (1), taking partial derivatives with respect to A and q, and making them equal to zero, we can acquire A and q as follows:

$$q = \frac{\sqrt{3}}{2},\ A = \frac{4}{5}\left(\varphi_0 - \frac{1}{3}\sqrt{-15r - 36\varphi_s^2}\right) \tag{5}$$

The physical details of all the parameters and the solving procedure of Eq. (3) spectrally implemented in the Fourier space can be referenced to Ref. [25]. Here, parameters used in the simulation are

$$(r, \varphi_0, \Delta x, \Delta y, \Delta t, \alpha, \beta) = (-0.6, 0.3951, \pi/4, \pi/4, 0.001, 20, 0.9), \tag{6}$$

where r is the dimensionless parameter relating to temperature, Δx and Δy are the grid-sizes and Δt is the time-step size. The values of parameters α and β are set in the elasticity response regimes of MPFC, the detailed relationship between the two parameters have been illuminated in Ref. [18].

2.2. Strain application and characterization

In trying to understand the length scales effect on the shear strain response, we need to have a common length scale parameter. For this purpose, we define the characteristic length scale as the length-to-height (x/y) aspect ratio of the specimen. In this work, the entire simulation domain is a rectangle scaled by $n\Delta x \times m\Delta y$, where n and m represent the number of lattice in x and y direction of the domain, respectively. The rectangle domain is divided into two parts. A small coexisting liquid boundary of width $100\Delta x$ is included on all four sides of the sample. The major reason for setting the liquid area is for the MPFC model cannot use free surfaces as in MD simulations to simulate deformation process. However, we can create free surfaces by choosing chemical potential to vary spatially over narrow strips near the solid-liquid interfaces of the system, as illustrated in Fig. 1. This is achieved by choosing values of r and φ_0 from the coexistence region of the hexagonal solid and liquid phase diagram [9,12].

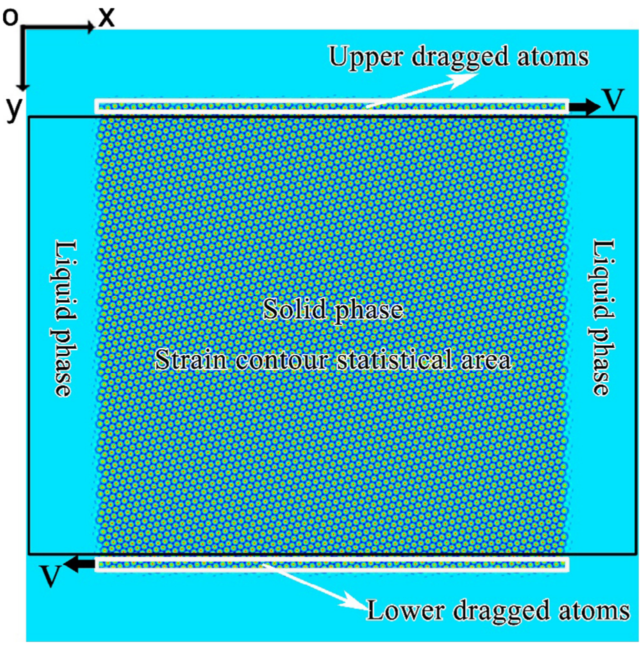

Fig. 1. Schematic illustration of simulation atom density field of a nano-single crystal specimen for the x/y aspect ratio of 1:1, where the coordinate axis is shown at the upper-left corner. The atoms within the white rectangle box are coupled to the external field. The light blue zone is liquid phase and black rectangle represents the statistical area of strain contour. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)