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Phase field model of deformation twinning in tantalum: Parameterization via molecular dynamics

Yijia Gu,[a] Long-Qing Chen,[a] Tae Wook Heo,[a] Luis Sandoval[b,*] and James Belak[b]

[a]*Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802, USA*
[b]*Condensed Matter and Materials, Lawrence Livermore National Laboratory, Livermore, CA 94550, USA*

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We present a phase field model to simulate the microstructure evolution during deformation twinning in tantalum. An order parameter, proportional to the shear strain, is employed to monitor the twinning process. The evolution of the order parameter is governed by a time-dependent Ginzburg–Landau equation, the parameters of which are determined by molecular dynamics with a model-generalized pseudopotential-theory potential. The twinning process is studied under a number of deformation conditions, and compared with the molecular dynamics counterpart.

Keywords: Deformation structure; Twinning; Phase-field model; Molecular dynamics

Twinning is an important deformation mechanism which, like slip, involves dislocation activity. It plays a prominent role in plasticity under extreme conditions of low temperature or rapid loading [1,2]. After nucleation at stress concentrators in the material, the twin lamellae start to thicken. A variety of modeling techniques have been used to study this growth process, as a complete description of the phenomenon spans many time and length scales, from molecular dynamics [3] to continuum micromechanical models [4].

In this work we present a phase field model (PFM) for deformation twinning in the body-centered cubic (bcc) metal tantalum, similar to the model developed by Heo et al. [5] for face-centered cubic aluminum. The phase field model is parameterized with values calculated using molecular dynamics (MD) with a model-generalized pseudopotential-theory potential (MGPT) potential [6], thus bridging atomic/molecular scale and mesoscale simulations. In this study we focus on a two-dimensional (2-D) model, although it can be easily extended to the general 3-D case by using the appropriate gradient energy coefficient, which is defined below.

Twinning in bcc metals takes place on $\{1\,1\,2\}$ planes along the $\langle 1\,1\,1\rangle$ direction. It also has directionality, which has been explained through the minimum shear hypothesis [7], from where there only are 12 possible twinning modes.

The PFM 2-D computational cell is shown in Figure 1, which describes the process of deformation twinning as seen on the plane of shear $(0\,1\,1)$ [2]. Under these specifications there are only two possible twinning modes, which we have called variant 1 $((\bar{2}\,1\,1)[\bar{1}\,\bar{1}\,\bar{1}])$ and variant 2 $((2\,1\,1)[1\,\bar{1}\,\bar{1}])$. The corresponding habit planes are related via a rotation of $\theta = 70.53°$. A new coordinate system (x', y', z') is defined along the $[\bar{1}\,0\,0], [0\,\bar{1}\,\bar{1}]$ and $[0\,\bar{1}\,1]$, respectively, which is also used in the MD simulations.

As has been previously established [5], 2-D simulations on the $(0\,1\,\bar{1})$ plane requires only two order parameters, η_1 and η_2; that is, two spatially dependent fields, $\eta_1(r)$ and $\eta_2(r)$, are sufficient to describe the twinning microstructures (12 for a general 3-D case). If defined in the specifically chosen local reference frame (the x-axis is defined along the twinning direction, the y-axis is defined along the direction normal to habit plane and the z-axis is determined by right-hand rule), the pure shear strain tensor is

$$\epsilon_{i,j}^{1,ref} = \begin{pmatrix} 0 & s/2 & 0 \\ s/2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{1}$$

and

* Corresponding author. E-mail: sandoval28@llnl.gov

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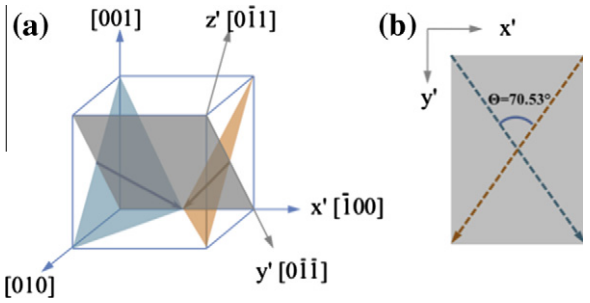

Figure 1. Crystallographic description of twinning for both variants (blue for variant 1, orange for variant 2). (a) Coordinate system set-up in a unit cell. (b) Configuration of the habit planes for both variants on the (0 1 1) plane. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

$$\epsilon_{i,j}^{2,ref} = \begin{pmatrix} 0 & -s/2 & 0 \\ -s/2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{2}$$

for variants 1 and 2, respectively, where $s = \sqrt{2}/2$ is the maximum magnitude of shear [2]. Transforming to the new coordinate system $(x'[\bar{1}\,0\,0], y'[0\,\bar{1}\,\bar{1}], z'[0\,\bar{1}\,1])$, we get, for both variants,

$$\epsilon_{i,j}^{1} = \begin{pmatrix} -\frac{s}{3} & \frac{s}{6\sqrt{2}} & 0 \\ \frac{s}{6\sqrt{2}} & \frac{s}{3} & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{3}$$

and

$$\epsilon_{i,j}^{2} = \begin{pmatrix} \frac{s}{3} & -\frac{s}{6\sqrt{2}} & 0 \\ -\frac{s}{6\sqrt{2}} & -\frac{s}{3} & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{4}$$

Assuming a linear dependence, the deformation strain tensor of variant p is then given by $\epsilon_{ij}^{(p)} = \eta_p \epsilon_{ij}^{p}$, where η_p is the order parameter describing the twinning process of variant p.

The evolution of order parameters is governed by the time-dependent Ginzburg–Landau (TDGL) equation,

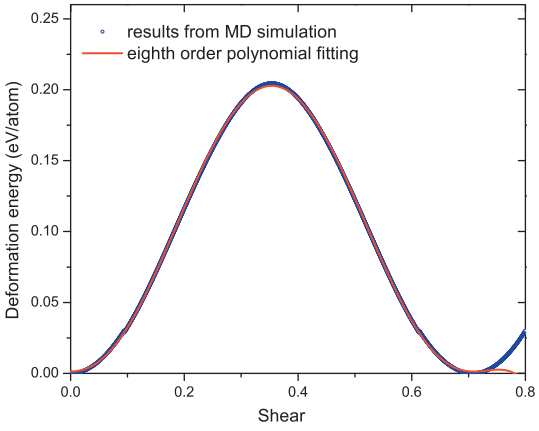

Figure 2. Deformation energy as a function of shear strain. The dashed line corresponds to an eighth-order polynomial fitting.

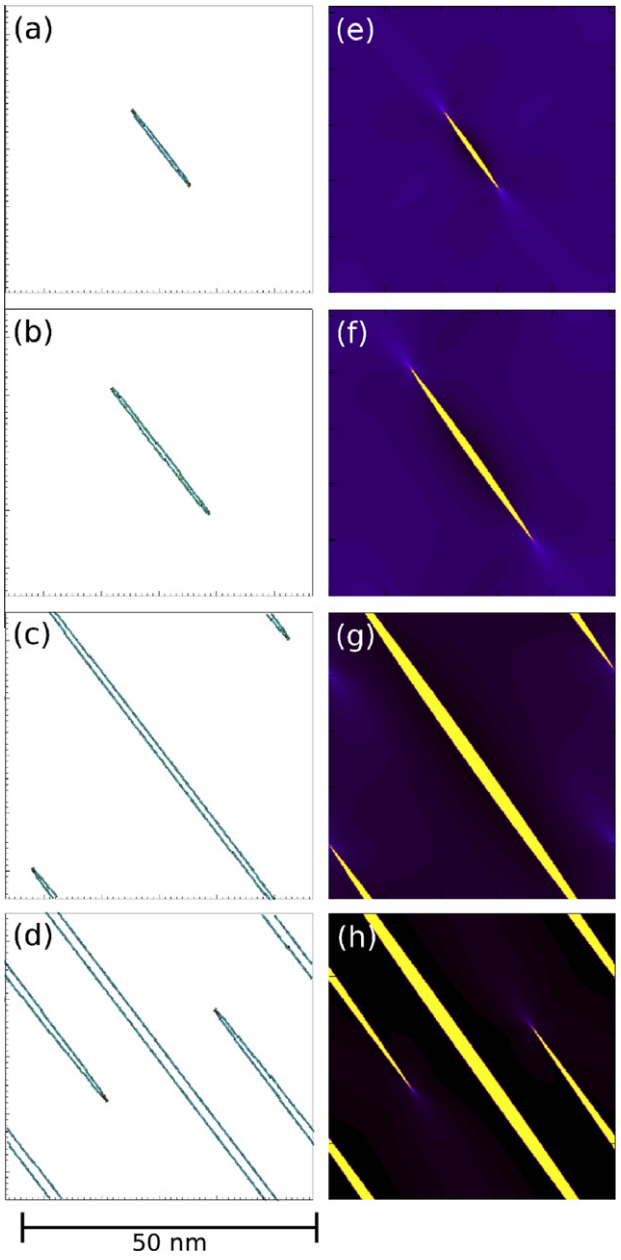

Figure 3. (a–d), MD simulations: (a) 2 ps, (b) 6 ps, (c) 18 ps, (d) 48 ps; (e–h), phase field simulations: (e) 1000 steps, (f) 5000 steps, (g) 15,000 steps, (h) 40,000 steps.

$$\begin{aligned} \frac{\partial \eta_p}{\partial t} &= -L\left(\frac{\delta F}{\delta \eta_p}\right) \\ &= -L\left(\frac{\partial f(\eta_p)}{\partial \eta_p} - \kappa_{p,ij}\nabla_i\nabla_j\eta_p + \frac{\partial E_{el}}{\partial \eta_p}\right) \end{aligned} \tag{5}$$

where t is time, F is the total free energy and L is the kinetic coefficient.

With the diffuse-interface description, the following volume integral gives the total free energy F of the system

$$F = \int_{\Omega}\left[f(\eta_1,\eta_2) + \sum_p \frac{\kappa_{ij}^{p}}{2}\nabla_i\eta_p\nabla_j\eta_p + \frac{1}{2}C_{ijkl}\left(\epsilon_{ij} - \epsilon_{ij}^{0}\right)\left(\epsilon_{kl} - \epsilon_{kl}^{0}\right)\right]\mathrm{d}V \tag{6}$$