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Orientation-dependent response of defective Tantalum single crystals

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ABSTRACT

Defective Tantalum monocrystals are expected to display a particularly rich behavior when stressed along different directions. Using molecular dynamics simulations, we model Ta monocrystals containing a single spherical void of different sizes, under uniaxial compression, for two empirical potentials. Differences on the yield point, dislocation generation and plastic heating are observed depending on the void size and stress direction, as distinct slip systems are activated, resulting in a variety of dislocation structures and mobilities.

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1. Introduction

Defects like dislocations, impurities, vacancies, etc., control metal plasticity, and determine applicability limits for technological applications. Voids, i.e. vacancy clusters, are ubiquitous in metals and they can arise during the manufacturing process [1,2], mechanical loading [3], or radiation damage [4,5]. Regarding mechanical loading, void nucleation is often considered the first stage of ductile fracture, and there are many studies focusing on void nucleation and growth at the nanoscale, specially for Face-Centered-Cubic (FCC) metals [6–12]. There is much less work focused on compression of nanovoids [4,13,14]. Atomistic simulations of FCC metals are carried out often partly due to large number of reliable empirical potentials for such metals [15]. Building accurate interatomic potentials for Body-Centered Cubic (BCC) metals is typically more challenging [16,17], but there is an increasing amount of work on voids in BCC metals [18–22]. Nevertheless, a large number of questions about the behavior of nanovoids under compression remain unanswered. New, detailed atomistic studies are needed in order to build reliable constitutive models which work at the nanoscale.

The mechanical behavior of materials with porosity has been treated with continuum-level constitutive model for decades, with the model by Gurson [23] leading to several improved and related models [24]. In general, these models do not take into account crystallographic orientation nor the effect of void size, with some notable exceptions [25–29]. Recent work by Bathia et al. [30] tries to improve on this for FCC Al monocrystals loaded along different directions and including voids.

In this study we also consider monocrystals but with BCC structure. Tantalum was chosen as a model BCC metal because of its technological relevance, and because it does not have thermodynamic phase transitions up to fairly high pressures and temperatures [16] unlike Iron [31]. Two different interatomic potentials are considered: the Extended Finnis–Sinclair (EFS) potential by Dai et al. [32], and the Embedded Atom Model (EAM) potential by Ravelo et al. [17]. Both potentials are of the EAM type, but we decided to call them in the above manner to be consistent with the style used by the scientific community and provide more clarity to the text. Ta monocrystals with a single void are subject to a compressive uniaxial load along the principal crystallographic directions, as an initial stage to study polycrystalline samples. Void size was systematically varied to obtain size-dependent yielding stress and compare to existing models.

2. Materials and methods

The simulations were performed using the molecular dynamics code LAMMPS [33]. Cubic single crystal samples with sides from 33 to 46 nm were generated with periodic boundary conditions along

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all directions. A spherical void with a radius r_v between 1.5 and 8 nm was introduced at the center of each sample, with the number of atoms between 2×10^6 and 6×10^6 to maintain the sample porosity below 2%. Atomic positions were relaxed using a conjugate gradient, and then were thermalized at 300 K for a few ps.

The use of nanovoids as effective dislocation sources has been extensively documented [13,19,20,34–40].

Homogeneous uniaxial compressive loading was applied to the samples, at a strain rate of $10^9 \, s^{-1}$. Atomistic simulations, where the integration time step typically is 1 fs, are limited to high strain rate loading. Such high strain rate is appropriate to study materials under shock waves, but it might also help understanding cases where other long-time scale events, like many thermally activated processes, could be neglected.

In order to study the effect of crystal orientation on plasticity mechanisms, loading was applied along the three principal crystallographic orientations, namely $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$. All simulations were carried out within the micro-canonical ensemble, monitoring the temperature evolution during the simulation to detect plastic heating. Dislocations emitted from a single void reached the periodic boundaries 1–3% strain after the initial nucleation. Larger strains are representative of a periodic array of closely spaced voids.

In order to evaluate possible changes in mechanical behavior due to different interatomic potentials, an Embedded Atom Model (EAM) potential for Ta by Ravelo et al. [17], was compared to the Extended Finnis–Sinclair (EFS) potential developed by Dai et al. [32]. Both potentials were fitted to high pressure results, as required for this study, but the EFS potential displays an artificial thermodynamic phase transition at ∼ 70 GPa [17]. The stress in our study is always well below that transition.

Visual analysis and rendering was carried out using Ovito [41] and VMD [42]. The Crystal Analysis Tool (CAT) developed by Stukowski et al. [43] was used to calculate dislocation densities, and detect other defects like vacancies and twins.

Since the material studied here is a single crystal of cubic BCC structure, for every potential the elastic behavior is described by the corresponding elastic constants, C_{11}, C_{12} and C_{44}. Several relationships between the elastic constants can be defined as follows:

The bulk modulus B, is defined as:

$$B = \frac{C_{11} + 2C_{12}}{3} \tag{1}$$

The Reuss-averaged shear modulus, G_{Reuss}, is defined as

$$G_{Reuss} = \frac{5(C_{11} - C_{12})C_{44}}{4C_{44} + 3(C_{11} - C_{12})} \tag{2}$$

The Voigt-averaged shear modulus, G_{Voigt}, is defined as

$$G_{Voigt} = \frac{C_{11} - C_{12} + 3C_{44}}{5} \tag{3}$$

The averaged shear modulus, G, is defined as the arithmetic mean over the Voigt-averaged and Reuss-averaged shear moduli

$$G = \frac{1}{2}(G_{Voigt} + G_{Reuss}) \tag{4}$$

Poisson's ratio, v, is defined as

$$v = \frac{3B - 2G}{2(G + 3B)} \tag{5}$$

Based on these quantities, we can define the Elastic modulus, E, as

$$E = 2G(v + 1) \tag{6}$$

While these calculations are very important for materials science in general, they fail to evidence the anisotropic behavior

suggested by the stiffness matrix. Therefore, we define X, the elastic anisotropy, as

$$X = \frac{2C_{44}}{C_{11} - C_{12}} \tag{7}$$

Finally, based on Meyers and Chawla [44], we can extract the orientation dependent elastic modulus by means of the following set of equations:

$$\frac{1}{E_{100}} = \frac{C_{11} + C_{12}}{(C_{11} + 2C_{12})(C_{11} - C_{12})} \tag{8}$$

$$\frac{1}{E_{110}} = \frac{C_{11}}{2(C_{11} + C_{12})(C_{11} - C_{12})} + \frac{1}{8C_{44}} \tag{9}$$

$$\frac{1}{E_{111}} = \frac{C_{11} + 2C_{12} + C_{44}}{3(C_{11} + 2C_{12})C_{44}} \tag{10}$$

The results for Eqs. (1)–(10) are summarized in Table 1. It must be noted that the EFS potential shows elastic moduli somewhat larger than the EAM potential, and more in agreement with experiments ($C_{11} = 264$ GPa, $C_{12} = 160$ GPa and $C_{44} = 82$ GPa) [45].

Orowan [46] expressed the plastic strain rate $\dot{\gamma}_p$, in terms of dislocations density ρ, and mean dislocation velocity $\bar{v}$, as:

$$\dot{\gamma}_p = b\rho_m \bar{v} \tag{11}$$

where b is the Burgers vector. Swegle and Grady [47] considered a modified equation particularly useful for high strain rate loading,

$$\dot{\gamma}_p = \frac{d\rho}{dt}b\bar{l} \tag{12}$$

where $\bar{l}$ is the average distance new dislocations move.

The temperature rise associated with plastic deformation can be expressed in a simplified fashion as:

$$\frac{dT}{dt} = \frac{\beta}{C}\tau(t)\dot{\gamma}_p \tag{13}$$

where C is the specific heat capacity, $\tau(t)$ is the time dependent shear stress, and β is an empirical parameter that represents the fraction of plastic work dissipated as heat [48].

3. Results

Fig. 1(a and d) shows the stress–strain curves for the each load direction and both potentials. As expected after the calculations shown in Table 1, the elastic behavior shown for each potential and each loading direction differs according to the orientation dependent elastic moduli. For instance, for [100] loading, the corresponding elastic modulus is higher for the EAM potential, while the EFS potential gives a higher modulus for [100] and [110] loading. This explains the different slopes in Fig. 1(a and d).

The large stress variation amongst the different crystalline directions in Fig. 1(a and d) is mostly due to elastic anisotropy. If we use S_{VM}/E_{hkl}, taking into account possible pressure induced

Table 1
Elastic constants and bulk properties calculated with Eqs.(1)–(10) for the EAM and EFS interatomic potentials at zero pressure. Experimental values for the elastic constants and the resulting calculated variables are also given ($C_{11} = 264$ GPa, $C_{12} = 160$ GPa and $C_{44} = 82$ GPa) [45].

Quantity	EFS	EAM	Quantity	EFS	EAM
C_{11} (GPa)	203.8	262.6	v	0.325	0.345
C_{12} (GPa)	143.5	160.7	E (GPa)	180	181
C_{44} (GPa)	91.3	81.8	X	2.09	1.66
B (GPa)	172.6	194.6	E_{100} (GPa)	120	140
G_{Reuss} (GPa)	63.5	65.8	E_{110} (GPa)	204	191
G_{Voigt} (GPa)	72.2	69.5	E_{111} (GPa)	231	215
G (GPa)	67.9	67.2			