Computational Materials Science 143 (2018) 126–132

Contents lists available at ScienceDirect

Computational Materials Science

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

Effect of symmetric and asymmetric tilt grain boundaries on the tensile behaviour of bcc-Niobium

Divya Singh, Avinash Parashar *

Department of Mechanical and Industrial Engineering, Indian Institute of Technology, Roorkee, India

ARTICLE INFO

Article history:
Received 3 October 2017
Received in revised form 2 November 2017
Accepted 3 November 2017

Keywords:
Molecular dynamics
Grain boundaries
Niobium
Dislocation

ABSTRACT

In this article, molecular dynamics based simulations were performed to investigate structure, energy and tensile behaviour of niobium (Nb) bi-crystals containing symmetric and asymmetric tilt grain boundaries. Six symmetric and four $\sum 5$ asymmetric tilt grain boundaries about $\langle 1\,0\,0 \rangle$ as tilt axis were generated in molecular dynamics based environment. Minimum grain boundary (GB) energy for each configuration was predicted, and subsequently the bi-crystal was subjected to tensile loading. The strengthening of bi-crystals in conjunction with dislocation evaluation was studied with the help of atomistic simulations, and results were further fitted with Taylor's work hardening expression. Simulations help in elucidating the effect of GBs and dislocations on the mechanical behaviour of Nb bi-crystals.

1. Introduction

Owing to superior properties such as low neutron cross-section, high ductility, hardness and corrosion resistance, zirconium (Zr) based alloys are commonly used as structural material in nuclear reactors. As a structural material for nuclear reactors, Zr is alloyed with niobium (Nb) to improve its mechanical properties [2]. Even for a small weight contribution, Nb is considered as an important constituent for the overall structural performance of Zr-Nb alloy.

In 1969, Tucker et al. [1] experimentally studied the mechanical behaviour of single crystals of Nb. In their work, formation of dislocation channels was reported in irradiated samples of Nb. Recently in 2017, Avinash and Divya [3] have studied the effect of irradiation on the tensile strength of single crystals of Nb. It was predicted from their numerical simulations that dislocation channelling plays an important role in governing mechanical strength of Nb, which was in agreement with the experimental observations made by Tucker et al. [1]. In 2008, Lewis and his team of researchers, experimentally studied the role of dislocations in polycrystalline Nb subjected to quasi-static tensile loading [5]. B. Joni et al. have employed X-ray diffraction techniques to study the effects of dislocation density and grain size on the mechanical properties of Nb [6]. Szkopiak in his work has determined the Hall-Petch parameters of Nb, namely Hall-Petch constant K and friction stress $\boldsymbol{\sigma_o}$ by grain size and extrapolation methods [7].

In polycrystalline materials, grain boundary (GB) structures and their spatial distribution, affects the mechanical properties at the macro level [8–10]. Plastic deformation in polycrystalline materials are assisted by grain boundary sliding, migration and nucleation of dislocations from grain boundary structures [20,21,25–27]. In addition to governing mechanical strength of polycrystalline materials, GB also acts as sinks for certain kind of point defects [11].

It has already been established that molecular dynamics based simulations represent an effective technique for the modelling of GB structures in metals and alloys [12–19]. Tschopp and McDowell [12,13] have studied asymmetric tilt GB structures in Copper and Aluminium. Ritnner and Seidmann [15] explored the structure and energies of twenty-one symmetrical tilt grain boundaries for fcc metals. In addition to these bi-crystals of single element, molecular dynamics based studies has also been performed with alloys [17]. As compared to fcc crystals, relatively fewer articles have been published on bcc bi-crystals [20,21]. Few examples are given by the works by Terentyev et al. [20] and Xuhang et al. [21] on structure, energy and strength of tilt grain boundaries in bcc α-iron.

So far, literature is almost mute on the effect of GB structure and energy on the tensile behaviour of bcc metals, in particular Nb. In this article, the authors have made an attempt to study the effect of GB structure on the mechanical response of bi-crystals of Nb. Symmetric as well as asymmetric tilt grain boundaries were considered in the simulations, and their effect on the tensile response was predicted for Nb bi-crystals. A relationship between dislocation density and yield strength was established to correlate the strength of bi-crystals of Nb.

* Corresponding author.
E-mail address: drap1fme@iitr.ac.in (A. Parashar).

https://doi.org/10.1016/j.commatsci.2017.11.005
0927-0256/

2. Simulation details

In this work, molecular dynamics based calculations were carried out in parallel Large Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), [23] whereas the post processing of dump files was performed in OVITO [24]. The reliability and accuracy of any molecular dynamics based simulations are entirely dependent on the type of potential used for estimating interatomic forces. All simulations in this work were carried out by utilizing the embedded atom method (EAM) potential proposed by Fellinger for Nb [22].

In this work, simulations were carried out in two stages, in the first stage, ten set of grain boundaries were generated and their corresponding energies were estimated, whereas in the second stage, the effect of GB configurations were studied with respect to their response to tensile loading.

A schematic of the simulation box is shown in Fig. 1. It depicts a bi-crystal, where â and ŵ denotes the direction of the common tilt axis and GB normal respectively, whereas the third direction is simply the cross product between ŵ×â. In order to study the effect of tilt grain boundaries on the tensile behaviour of Nb, six symmetric boundaries with different sigma coincidence and four asymmetrical GBs tilted along ⟨1 0 0⟩ axis with equal coincidence site lattice (CSL) ∑5 were generated in the molecular dynamics based environment. The modelling details of GB with respect to each mis-orientation angle (θ), sigma (∑) values, inclination angle (Ø) and GB planes are tabulated in Tables 1 and 2 for symmetrical and asymmetrical tilt GBs respectively. In the case of symmetric tilt boundaries, the GB plane remains the same for both the crystals, while it differs in bi-crystals containing asymmetric grain boundaries. In order to avoid any edge effects periodic boundary conditions were imposed in all the principal directions. The size of the simulation box was kept large enough to avoid any image interactions between the grain boundary structures.

In order to achieve minimum energy atomic configuration for symmetrical as well as asymmetrical GB's, conjugate gradient algorithm in conjunction with volume relaxation and rigid body translation were employed. After achieving minimum energy configuration, equilibration at desired temperature was performed (1K or 300 K) for 50 pico-seconds (ps) with a time step of 0.001 ps. During equilibration as well as in loading phase, simulation box was subjected to NPT ensemble (Number of atoms, pressure and temperature constant). In NPT ensemble, Nose-Hoover thermostat and barostat was used for controlling temperature and pressure respectively. Stress calculations were performed with the help of virial stresses [4] provided in Eq. (1)

$$\sigma_{ij}^{a} = \frac{1}{\Omega}\left(\frac{1}{2}m^{a}v_{i}^{a}v_{j}^{a} + \sum r_{\alpha\beta}^{j} f_{\alpha\beta}^{i}\right) \tag{1}$$

where

i,j = indices of cartesian coordinate
Ω = atomic volume of atom a
α, β = atomic indices
m^a = mass of atom a
v^a = velocity of atom a
$r_{\alpha\beta}$ = distance between atoms α and β
$f^i_{\alpha\beta}$ = force on α atom due to β atom in direction i

The microstructure evolution in conjunction with dislocation nucleation was studied with the help of dislocation extraction algorithm (DXA). Easy movement of dislocations helps in improving the ductility at the expense of material strength. During plastic deformation, as number of dislocations increases, more and more dislocations start interacting with each other, which causes impediment of dislocation motion, that further improves the strength of the material. Such a strengthening mechanism is known as *forest strengthening*. The flow stress for forest strengthening is correlated with the dislocation density by the Taylor's work hardening expression [6].

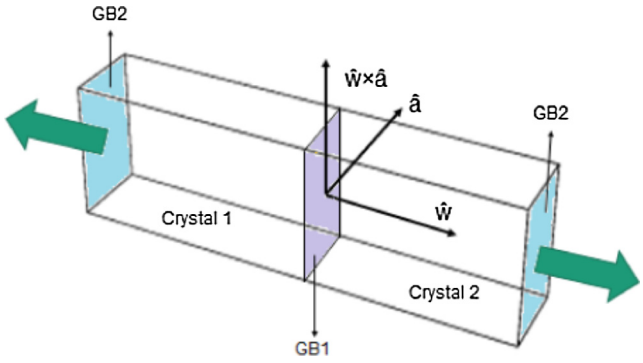

Fig. 1. Schematic of simulation box showing grain boundaries, three principle directions and loading direction.

$$\sigma_y = \sigma_o + \alpha MGb\sqrt{\rho} \tag{2a}$$

$$\sigma_y = \sigma_o + \delta\sigma_y \tag{2b}$$

$$\delta\sigma_y = \sigma_y - \sigma_o = \alpha MGb\sqrt{\rho} \tag{2c}$$

Here, $\delta\boldsymbol{\sigma_y}$ is the increase in the strength due to forest dislocations, $\boldsymbol{\sigma_y}$ and $\boldsymbol{\sigma_o}$ are the yield strength and friction stress, respectively. On the other hand, alpha (α) and M (Taylor's factor) are taken as constants with 1.1 and 3.1 as their respective values. **G** is the shear modulus, **b** is the length of the burger's vector and **ρ** is the dislocation density. The dislocation density is defined as number of dislocations per unit volume of the crystal. Due to computational limitations associated with molecular dynamics based simulations, high strain rate loading was used in the simulation that accounts for the high yield strength.

3. Results and discussions

As mentioned in the previous section, simulations were performed in two stages. In stage one, minimum energy atomic configuration in conjunction with GB energies were predicted for different set of symmetrical as well as asymmetrical tilt grain boundaries of Nb. Subsequently, after achieving the minimum energy structure for the grain boundaries, bi-crystals of Nb were subjected to tensile loading as illustrated in the schematic in Fig. 1.

3.1. GB structures and energies

In this stage of simulations, symmetrical as well as asymmetrical tilt grain boundaries were generated along the ⟨1 0 0⟩ as the tilt axis. Snapshots of the simulation box containing symmetrical grain boundaries are shown in Fig. 2, whereas the corresponding GB energies are plotted in Fig. 3. In Fig. 2, blue[1] colour atoms corresponds to bcc crystal structure in Nb, whereas the coloured atoms in the centre are representing the GB.

It can be inferred from Fig. 3 that at a mis-orientation angle of 36.86° a saddle occurs in the GB energy curve for ∑5 ⟨3 1 0⟩ GB plane. The GB structure corresponding to minimum energy (θ = 36.86°) is most coherent and uniform as seen in Fig. 2b. The GB structure or configuration for higher energy is more disordered,

[1] For interpretation of colour in Fig. 2, the reader is referred to the web version of this article.