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Molecular dynamics investigation of c-axis deformation of single crystal Ti under uniaxial stress conditions: Evolution of compression twinning and dislocations

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ABSTRACT

Twinning plays an important role on the microstructure evolution of HCP metals. In this work, we perform c-axis compression of single crystal Ti under uniaxial stress conditions using molecular dynamics simulations. The objective is to demonstrate activation and evolution of compression twins along with dislocations when Ti single crystals are loaded in uniaxial stress conditions using two commonly utilized interatomic potentials. We find that activation of only $\{10\bar{1}1\}$ compression twins with the Kim potential is inconsistent with the Schmid criterion while activation of both $\{10\bar{1}1\}$ and $\{11\bar{2}2\}$ compression twins with the Hennig potential is consistent with the Schmid criterion. Twin variants activated do not contribute equally to the total twinned volume even with equal Schmid factor for both potentials and thereby demonstrating inability of the Schmid criterion to predict dominance and evolution of twin variants. The Kim potential shows large amount of dislocation density in comparison to the Hennig potential. The strain rate sensitivity on activation of compression twin systems is observed with the Hennig potential. The study can be utilized to further investigate the evolution of compression twins required to develop/improve twin volume fraction evolution laws for crystal plasticity finite element simulations.

1. Introduction

Hexagonal-close-pack metal at ambient temperature and pressure conditions, Titanium (typically referred to as α-Ti) is used in different industries primarily because of its light weight, high strength and stiffness apart from being bio-compatible and being resistant to wear and corrosion. Due to its HCP crystal structure, it has a high propensity for deformation twinning compared to the dislocation slip when subjected to c-axis loading. Deformation twinning is an important plastic deformation mode in HCP metals [1,2] and plays an important role in texture evolution [3], strain hardening [4,5], ductility and fracture strength [6]. Based on the nature of the c-axis loading, the deformation twins are categorized as tension twins (for c-axis extension) and compression twins (for c-axis contraction). The most commonly reported tension twins are $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ and the compression twins are $\{11\bar{2}2\}$, $\{11\bar{2}4\}$ and $\{10\bar{1}1\}$ [6–8]. The $\{11\bar{2}2\}$ compression twins are most frequently observed at ambient temperature and pressure conditions [9–11] whereas $\{11\bar{2}4\}$ are reported to activate at low temperatures [12]. The $\{10\bar{1}1\}$ twins activate at elevated temperatures [9] and at room temperatures (have been observed in micro-pillar compression experiments on single crystal titanium alloy [11] and dynamic compression experiments on commercially pure titanium [13]).

The twinning-induced plastic deformation in HCP metals such as Mg and Ti are commonly investigated using Crystal plasticity finite element (CPFE) simulations [5,14]. In these simulations, the twin volume fraction is computed and tracked on each twin system at each Gauss point. When the overall twin volume fraction at any Gauss point reaches a critical value, the volume associated with that Gauss point is reoriented based on the dominant twin variant of a twin system. In this approach, it is assumed that the activation and evolution of twin systems and their variants follow the Schmid criterion. In fact, the activation of twin systems in most of the cases is found to follow the Schmid criterion. However, ability of the Schmid factor to predict evolution and dominance of twin variants is still not clear. This is primarily because the in situ measurements of twin variant evolution are major challenges in experiments. In this regard, atomistic simulations can serve as a useful resolution to investigate the evolution and dominance of twin variants under

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the applied loading conditions [15]. Note that such information can be useful to improve the twinning evolution laws for predictive CPFE simulations.

Recently, Rawat et al. [16] compared the deformation behaviour of Ti single crystal under uniaxial strain condition using four commonly utilized interatomic potentials: Finnis-Sinclair [17], embedded atom method (EAM) [18], 2NN modified embedded atom method (MEAM) [19] and spline-based modified embedded atom method [20] potentials and concluded that the Kim potential [19] should be considered for c-axis compressive uniaxial strain conditions. The superiority of the MEAM potentials over the embedded atom method and Finnis-Sinclair potentials is also established in literature since these potentials account for angular dependence of electron density to account for bond bending, have stacking fault energies (SFEs) (SFE^{Kim} = 213 mJ m^{-1} [19], SFE^{Hennig} = 170 mJ m^{-1} [20]) near the experimentally observed value (300 mJ m^{-1} [1]) and are also able to reproduce c/a ratio as well as other properties simultaneously. Note that the SFE plays an important role on the activation of preferred slip/twin systems as well as dislocation mobility [21]. The EAM [18] and Finnis-Sinclair [17] potentials with very low stacking fault energies (SFE^{Mishin} = 56 mJ m^{-1} [18] and $SFE^{Ackland}$ = 64 mJ m^{-1} [17]) may not be appropriate to predict the deformation response of Ti as they may not be able to reproduce the realistic dislocation core structure [22–24]. Thereby only MEAM potentials are being considered in this work to study the response of Ti single crystal under uniaxial stress type of loading situation. In the MEAM formalism, the pair interactions are computed as a function of nearest-neighbour distance from the known values of total energy and the embedding function. The original 1NN (NN refers to nearest-neighbour) MEAM which considers only first nearest-neighbour distance to compute the electron densities was found to have some structural stability issues [25]. In the 2NN MEAM potential [19], the second nearest-neighbour interactions are considered to compute the electron densities to resolve the structural stability issues. The spline-based MEAM [20] considers the cubic spline functions to compute the total energy of the system and the electron density described in this potential removes the constraint of fixed angular character.

In this work, we simulate c-axis compression of perfect single crystal Ti at room temperature under uniaxial stress condition using two commonly utilized interatomic potentials [19,20] with an objective to investigate the deformation behaviour of single crystal Ti. It should be noted that the uniaxial stress conditions are different from the uniaxial strain conditions [26] (highlighted in our previous publication [16]). The uniaxial stress conditions are representative of loading conditions which occur in static compression experiments using Universal Testing Machine as well as dynamic compression experiments using Kolsky bar [27]; whereas uniaxial strain conditions are representative of shock loading situations [26] in high velocity impact experiments [28] or by laser ablation [29]. Fig. 1 shows a representative diagram for the two cases for ease of understanding of the readers.

For uniaxial stress conditions, the pressure along X- and Y-directions is kept at 0 bar and thereby the material can change shape and size along those directions; whereas for uniaxial strain conditions the material is constrained to change shape and size along X- and Y-directions and thereby stresses can originate in these directions. Note that since there are no experimental investigations at ultra high strain rates, as carried out in this manuscript, it is difficult to comment on suitability of one individual MEAM potential over the other. In this manuscript, we present the response of single crystal Ti with both available MEAM potentials under uniaxial stress conditions and expect that the results would be compared and validated in future by experimental investigations.

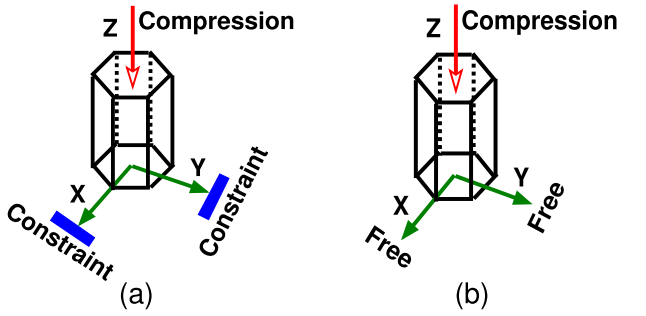

Fig. 1. (a) C-axis compression under uniaxial strain conditions [16]. (b) C-axis compression under uniaxial stress conditions.

2. Computational method

We use LAMMPS [30] to simulate the c-axis compression of perfect single crystal titanium under uniaxial stress condition ($\sigma_{zz} \neq 0$, $\sigma_{xx} = \sigma_{yy} = 0$). The simulation domain contains 4.6 $\times$ 10^5 atoms and each side length of the domain is 20 nm. The X-,Y- and Z-directions of the simulation domain correspond to $\langle 2\bar{1}\bar{1}0\rangle$, $\langle 01\bar{1}0\rangle$ and $\langle 0001\rangle$, respectively. The periodic boundary conditions are used in each direction and velocity-Verlet algorithm is used to integrate the equation of motion with a timestep of 2 femto-second. We use the spline-based modified embedded atom method (MEAM) potential [20] (henceforth being referred to as the Hennig potential) and the 2NN-MEAM potential [19] (henceforth being referred to as the Kim potential) to study the comparative deformation behaviour of perfect single crystal titanium. To control the temperature and pressure, Nose-Hoover thermostat and barostat are used. The system is first equilibrated at 300 K and 0 bar pressure using an NPT ensemble up to 40 ps and then a strain rate of 10^9 s^{-1} is applied along the Z-axis (c-axis) to compress the system at a constant temperature of 300 K. The pressure along the X- and Y-directions is kept at 0 bar using an NPT ensemble thereby allowing the material to change shape and size along these directions. The simulations at 10^9 s^{-1} strain rate are performed to save computational time. To study the role of applied strain rate on the results, we also perform simulations at 10^8 s^{-1} strain rate. The atomic data is then post-processed using basal plane vector analysis [31] and crystal analysis tool (CAT) [32]. The results are visualized in Ovito [33].

3. Results and discussion

3.1. Stress-time profile

Fig. 2 shows the axial stress as a function of time for single crystal titanium deformed at 10^9 s^{-1} strain rate with the Kim [19] and the Hennig [20] potentials. Typically a sharp fall in stress indicates stress relaxation due to defect nucleation in the material. Thereby it is observed that since the peak stress for the Kim potential [19] is very high (~2 times) in comparison to that obtained with the Hennig potential, higher stress is required for the nucleation of defects with the Kim potential compared to that with the Hennig potential. In fact, this type of behaviour is also expected since the Kim potential has high stacking fault energy in comparison to the Hennig potential.

Interestingly, the Kim potential shows only a single peak in the stress-time profile, whereas the Hennig potential shows double peaks in the stress-time profile (Fig. 2). The presence of double peaks with the Hennig potential indicates that the microstructural evolution with the Hennig potential is quite different from that