Computational Materials Science 141 (2018) 302–312

Contents lists available at ScienceDirect

Computational Materials Science

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

Evolution of tension twinning in single crystal Ti under compressive uniaxial strain conditions

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ARTICLE INFO

Article history:
Received 8 May 2017
Received in revised form 22 September 2017
Accepted 23 September 2017

Keywords:
Deformation twinning
Single crystal
Molecular dynamics simulations
HCP metals
Titanium

ABSTRACT

We perform molecular dynamics simulations to study the evolution of tension twinning in single crystal Ti under uniaxial strain conditions. The objective is to understand the evolution trends of twin volume fraction as well as number of twins and express them in terms of the individual twin dynamics. The compressive strain applied along $\langle 2\bar{1}\bar{1}0\rangle$ and $\langle 01\bar{1}0\rangle$ directions leads to the activation of $\{10\bar{1}2\}$ twin variants. We find that the activation of twin variants follows the Schmid criterion. However, they do not activate at the same time even with equal Schmid factor indicating the stochastic nature of the twin variant activation. For the case where four variants activate (loading along $\langle 2\bar{1}\bar{1}0\rangle$ direction), high nucleation events occur compared to the case where only two variants activate (loading along $\langle 01\bar{1}0\rangle$ direction). The activated variants in each case do not evolve with same rate even with equal Schmid factor and a clear dominance of twin variants is observed. For the case where only two variants activate, average twin growth rate and overall twin volume fraction are high compared to the case where four variants activate. A correlation between the number of activated variants and the overall twin volume fraction is observed. The size distribution of the nucleated twins follows the power law function. The expressions provided for overall number of twins and overall twin volume fraction can serve as a basis to develop the physics-based twin evolution laws to model twinning at higher length scales.

1. Introduction

The $\{10\bar{1}2\}$ twins (known as tension twins) in HCP metals such as Ti and Mg are commonly observed at room temperature under c-axis extension and play an important role on texture evolution [1], strain hardening [2] and damage tolerance [3]. There are six possible variants of $\{10\bar{1}2\}$ twins which reorient the crystal nearly perpendicular to the parent matrix (85.03° for Ti [4]) in six possible ways. It is observed that the $\{10\bar{1}2\}$ twins can consume the entire parent matrix under some suitable loading situations [5].

To understand the twinning induced plasticity and texture evolution, deformation twinning is commonly modelled using crystal plasticity finite element (CPFE) simulations [6–13], viscoplastic self-consistent (VPSC) and elastic viscoplastic self-consistent (EVPSC) simulations [14–18]. Typically in these simulations, it is assumed that the activation and evolution of twins follow the Schmid law and the twinning is modelled by tracking the twin volume fraction (TVF) on each twin system. Once the overall TVF reaches a critical value, the grain is reoriented based on the commonly used predominant twin reorientation (PTR) scheme [19]. In this regard, Kadiri et al. [5] based on their experimental results suggested that the PTR scheme [19] can be accurate for twin variants with non-equal Schmid factors. However, there may be situations where the twin variants may have nearly equal Schmid factors and comparable twin volume fraction. In those situations, PTR scheme [19] may not work well since it will neglect the twin variants with comparable twin volume fraction and affect the texture of the material which in turn affects the material response. Moreover, in the CPFE approaches [6–12], the discrete twins and their interactions are not handled, i.e. the population and volume fraction of individual twins are not computed at each material point in a given finite element. Instead the twin variant volume fraction, a collective behaviour of individual twins, is computed and tracked. While it is known that the twin-twin interactions affect the properties such as strain hardening [2,5], therefore, there is a need to develop physics-based evolution laws for twinning.

Experiments have revealed some of the important aspects of tension twins such as twin boundary deviation from $\{10\bar{1}2\}$ twin plane [20,21], role of twin-twin interaction on the nucleation and growth rates of twins [5]. However, it is very difficult to investigate

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https://doi.org/10.1016/j.commatsci.2017.09.041
0927-0256/

the individual twin dynamics through experiments since nucleation and growth processes of twins are difficult to separate in experiments. In this regard, the classical molecular dynamics (MD) simulations can serve as a useful tool to develop a fundamental understanding of twinning evolution in HCP single crystals and can provide useful information for continuum simulations. For example, the twin variant level information at any material point (or Gauss point) in a finite element in CPFE simulations [6–12] can be obtained using MD simulations [22].

Recent MD simulations investigate the activation and evolution of $\{10\bar{1}2\}$ twins at atomistic scale with a focus on role of crystal orientations [23], loading conditions [22,23], pre-existing defects [22–24], initial temperature [24] and basal-prismatic boundary [25]. However, there is limited work on the evolution of tension twins using MD simulations which focuses on the individual twin dynamics and twin variant evolution. Very recently, Rawat et al. [22] investigated the evolution of $\{10\bar{1}2\}$ twin variants in single crystal Mg (c/a = 1.624) under different loading conditions using MD simulations and found that the activation of $\{10\bar{1}2\}$ twin variants follows the Schmid law. They also found that the activated twin variants did not contribute equally to the overall TVF even with equal Schmid factor and concluded that the Schmid factor cannot dictate the evolution and dominance of twin variants. Note that those simulations [22] were performed at low temperature (5 K) to get negligible thermal contribution to the activation and evolution of tension twins and in those simulations, either both lateral directions were free to move under the applied strain or one of the directions was free to move and other one was fixed. In this work, we choose Ti (c/a = 1.58) as a test material to investigate the twin evolution dynamics under uniaxial strain conditions [26,27] and perform simulations at 300 K temperature to include the thermal contribution to the activation and evolution of tension twins. It should be noted that uniaxial strain conditions [27] typically observed in shock loading of materials obtained through high velocity impact experiments and/or laser ablation [26,28,29] are different from uniaxial stress conditions [30] obtained in Kolsky bar experiments [31]. In an uniaxial strain situation, the stress state is three-dimensional and can be decomposed into a hydrostatic (responsible for change in volume of the material) and a deviatoric component (responsible for plastic deformation and associated substructure generation).

Apart from the variant level information at any material point in a given finite element in CPFE simulations [22]; from a continuum point of view, one would also be interested to know: Does twinning consume the entire parent HCP structure? How the overall twinned volume distribute over twins, i.e. Does twinning evolution take place through the evolution of few twins or many twins? Do all nucleated twins make significant contribution to the overall twinned volume? Does activation of twin variants follow Schmid criterion? Do the twin variants with equal Schmid factor activate at the same time? Do all variants activated contribute equally to the overall twinned volume? Can Schmid factor analysis predict the evolution and dominance of twin variants? What is the role of nucleation, growth and coalescence/detwinning processes on the evolution of twin number density? Do the number of activated twin variants and twin number density affect the overall twinned volume at saturation? Does the twin nucleation order play any role on the growth of the twins? Do the volume of the nucleated twins follow any distribution function? These and allied questions can help in understanding the twin evolution dynamics under the applied loading conditions and can serve as a basis to develop the physics-based evolution laws for twinning in HCP metals.

The objective of the present work is to investigate the evolution of tension twins in single crystal Ti under uniaxial strain conditions at room temperature using two well known inter-atomic potentials, Kim [32] and Hennig [33]. To our knowledge, there is no work on Ti using MD simulations which explores the evolution of $\{10\bar{1}2\}$ twins and their variants under uniaxial strain conditions as well as other loading conditions. In this work, we consider the perfect single crystal of Ti which represents an ideal situation where there are no pre-existing defect (twin) nucleation sites and each point in the lattice serves as the nucleation sites for the defects. Single crystal idealization is also applicable to represent bulk region within a large sized grain of the material. The role of pre-existing defects as well as grain boundaries, which may serve as defect (twin) nucleation sites, have been kept outside the scope of this manuscript. It is known that the twinning in HCP metals takes place through the nucleation as well as evolution of the twins. This entire process can be understood from the following two aspects: how twinning occurs (i.e. exploring the twin nucleation mechanism) and how twinning evolve (i.e. exploring the twin evolution dynamics) under the applied loading conditions. This manuscript focuses on the latter part, i.e. understanding the twin evolution dynamics which is required to improve the twin evolution laws for the crystal plasticity finite element simulations.

2. Computational method

We perform compression of perfect single crystal titanium under uniaxial strain conditions [27] using an open source molecular dynamics code, LAMMPS [34]. The simulation domain contains 4.6×10^5 atoms with a side length of 20 nm in each direction. 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 all three directions and velocity-Verlet algorithm is used to integrate the equations of motion with a timestep of 2 femto-second. Nose-Hoover thermostat and barostat are used to control the temperature and pressure of the system. We use two well known modified embedded-atom method inter-atomic potentials for Ti: Kim et al. [32] (henceforth will be referred as Kim) and Hennig et al. [33] (henceforth will be referred as Hennig). The system is first equilibrated at 300 K and 0 bar pressure using an NPT ensemble up to 40 ps. After equilibration, a nominal strain rate of 10^9 s^{-1} is applied to deform the system at a constant temperature of 300 K using an NVT ensemble. The simulations at 10^9 s^{-1} strain rate are performed to save computational time. The atomic data is then post-processed using the crystal analysis tool (CAT) [35] and results are visualized in Ovito [36].

We simulate two cases of loading conditions under uniaxial strain conditions: (*a*) compressive strain is applied along $\langle 2\bar{1}\bar{1}0\rangle$ direction which results in an extension of the c-axis and hence leads to the activation of tension twins (*b*) compressive strain is applied along $\langle 01\bar{1}0\rangle$ direction which also results in the extension of the c-axis leading to the activation of tension twins. For deformation under uniaxial strain conditions, the constraints are applied on $\langle 01\bar{1}0\rangle$ (global Y) and $\langle 0001\rangle$ (global Z) directions for case A and $\langle 2\bar{1}\bar{1}0\rangle$ (global X) and $\langle 0001\rangle$ (global Z) directions for case B so that no strain can develop along these directions during the applied strain.

The loading conditions simulated in this work are summarized in Fig. 1.

3. Results and discussion

3.1. Misorientation angle distribution

Fig. 2 shows the distribution of c-axis misorientation at a given time point for both loading conditions with Kim and Hennig potentials.