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Is the pinning of ordinary dislocations in γ-TiAl intrinsic or extrinsic in nature? A combined atomistic and kinetic Monte Carlo approach

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Abstract

We address the question of the observed pinning of $\frac{1}{2}\langle 1\,\bar{1}\,0]$ ordinary screw dislocations in γ-TiAl, which leads to the characteristic trailing of dipoles in the microstructure. While it has been proposed that these may be variously intrinsic or extrinsic in nature, we are able to rule out the former mechanism. We do this by means of very large scale, three-dimensional atomistic simulations using the quantum mechanical bond order potential. We find that the kink-pair formation energy is large – 6 eV – while the single kink migration energy is conversely very small – 0.13 eV. Using these, and other atomistically derived, data, we make kinetic Monte Carlo simulations at realistic time and length scales to simulate dislocation mobility as a function of stress and temperature. In the temperature range of the stress anomaly in γ-TiAl, we determine whether one or several of the pinning and unzipping processes associated with generation of jogs are observed during our simulations. We conclude that the pinning of ordinary dislocations and anomalous mechanical behaviour in γ-TiAl must be attributed to a combination of extrinsic obstacles and extensive cross-slip in a crystal containing impurities.

Keywords: Modelling; Dislocation mobility; Monte Carlo techniques; Titanium alloys

1. Introduction

It is well known that the deformation behaviour of γ-TiAl is complex due to the tetragonality of the $L1_0$ structure. The γ phase of TiAl can deform by several deformation modes: glide of ordinary dislocations, glide of superlattice dislocations and twinning [1]. The $\mathbf{b} = \frac{1}{2}\langle 1\,\bar{1}\,0]$ ordinary dislocations in deformed TiAl alloys exhibit a unique morphology consisting of numerous pinning points along the dislocation line aligned roughly along the screw dislocation direction, and bowed-out segments between the pinning points [1]. Post mortem TEM analyses [2–4] have shown that the screw segments separated by pinning points are lying in different parallel (1 1 1) planes as a result of a cross-slip mechanism. Extensive cross-slip was also observed in in situ straining experiments [5]. Yield stress anomaly (increase of the yield stress with temperature) has been observed in γ-TiAl compounds and ascribed to the $\frac{1}{2}\langle 1\,\bar{1}\,0\rangle\{1\,1\,1\}$ slip system [3,6,7]. There is compelling microscopic evidence that pinning plays a prominent role in the anomalous mechanical behaviour. The determination of the subsequent cusp unpinning mechanism is of fundamental importance in the interpretation of the stress anomaly.

Deep cusps and the trailing of dipoles suggest that the dislocations have many jogs. At the microscopic scale, the pinning points have been analysed as jogs aligned along the screw direction, whose density increases with temperature in the domain of the stress anomaly [8,9]. The exact nature of the obstacles developed on these cross-kinks seems to be controversial. Viguier et al. [3] and Sriram et al. [4] have concluded that the pinning points are formed as a result of intrinsic processes involving single or double cross-slip mechanisms, leading to formation of jogs. The three-dimensional (3-D) structure formed during collision of kinks during their lateral propagation cannot move in the direction of the dislocation glide. Explanations based

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on the activation of cross-slip suffer, however, from not explaining satisfactorily a number of experimental results:

1. Non-screw ordinary dislocations, Shockley dislocations involved in twinning and superlattice dislocations are also anchored at many points [10–13].
2. Ordinary dislocations moving in the same plane are able to anchor at exactly the same location in the sample [5].
3. An annealing treatment which precipitates interstitial atoms in excess decreases the density of cusps and debris [2].

To explain these experimental results, it was concluded that pinning points are extrinsic in nature and due to some chemical heterogeneity [2,11,14]. Messerschmidt et al. [10] and Morris [15] have ascribed these pinning points to small extrinsic obstacles like oxygen atoms or Al_2O_3 precipitates.

Understanding the glide mechanism of ordinary dislocations in different stress and temperature ranges can help us to determine which of its main features is likely to account for the strength anomaly of γ-TiAl. In addition, the behaviour of these ordinary dislocations deserves particular attention since they are responsible for most of the deformation in two-phase lamellar TiAl alloys [16–19].

The present work aims at exploring the mobility of $\frac{1}{2}\langle 1\bar{1}0]$ ordinary screw dislocations in γ-TiAl through simulation of the specific mechanisms of motion of an individual dislocation in the $L1_0$ structure.

Due to the high Peierls barrier [16,20], the motion of ordinary screw dislocations in TiAl is believed to be controlled by nucleation, migration and annihilation of kinks. When the stress on a dislocation is lower than its Peierls stress, the dislocation line stays at rest in a given lattice position, interrupted by the thermally assisted process of kink-pair nucleation. The separation of kinks under the influence of stress and thermal activation results in translation of the entire dislocation line to the next lattice position. The overall dislocation movement is a cumulative effect of a large number of individual kink events.

Dislocation dynamics (DD) simulations [21,22] employ simple rules that dictate the motions of dislocations which are represented as interconnected small straight segments in an elastic continuum connected through nodes. Local stresses resulting from applied loading and internal stresses are computed on each of those segments. The dynamics of dislocation motion is thus reduced to the dynamics of the nodes prescribed by the mobility rules. Such a description replaces the true kink dynamics of dislocation glide with a mean field measure of the average mobility of a dislocation line. The reliability with which the DD simulations mimic the plastic behaviour of the crystal depends on the accuracy of the mobility rules.

In order to overcome these limitations and to obtain a more realistic description of the dynamics of a dislocation line over long time scales, we carry out kinetic Monte Carlo (kMC) simulations of the mobility of $\frac{1}{2}\langle 1\bar{1}0]$ dislocations. Several researchers have performed kMC studies of dislocation behaviour to provide a more realistic link between kink dynamics and the averaged dynamics of a dislocation line [23–25]. The advantage of this approach is that it replaces arbitrary assumptions about the nature of dislocation mobility with input based upon microscopic understanding. In addition, kMC can achieve extended time scales for simulation of the dislocation mobility. kMC simulations use atomistic results for the nature of the core energetics, short-range dislocation segment interactions and rate theory to simulate dislocation mobility as a function of stress and temperature.

In our simulations we assume that the ordinary dislocation moves by the kink mechanism through adjacent Peierls valleys. We examine ordinary dislocation mobility in TiAl at fixed stresses and temperatures based upon atomistic input. The rates of kink-pair nucleation and kink migration events are expressed in terms of their respective energy barriers, which are computed using atomistic simulation techniques. The kMC model allows dislocations to cross-slip onto secondary glide planes. Thus, motion of screw dislocations becomes three-dimensional and can involve a number of unusual mechanisms affecting dislocation mobility. In the temperature range of the stress anomaly, we check whether one or several of the above-mentioned pinning and unzipping processes associated with generation of jogs are observed during simulations.

2. kMC model

Ordinary screw dislocations in TiAl do not dissociate into a planar structure due to the high energy of the complex stacking fault (CSF) in γ-TiAl [20]. Instead, the non-planar core of these dislocations spreads symmetrically on two cross-slip $\{1\,1\,1\}$ planes (Fig. 1) and their glide is not confined to a single glide plane. Cross-slip should readily occur by which screw dislocations change their glide planes. In fact, each screw dislocation segment can nucleate kink-pairs on either of the two $\{1\,1\,1\}$ planes.

The kMC model does not consider any details of the core structure. It focuses on dislocation motion on length and time scales far greater than those of atomistic simulations. The key idea of kMC is to treat dislocation motion as a stochastic sequence of discrete rare events whose mechanisms and rates are computed within the framework of transition state theory. Dislocations are represented as interconnected small straight segments in an elastic continuum. Local stresses resulting from applied loading and internal stresses are computed on each of those segments.

In the present model, we study the ordinary screw dislocation represented by a piecewise straight line stretched along the $[1\bar{1}0]$ direction. While the dislocation has, on average, a screw orientation, it consists of screw (S) and edge (E) dislocation segments such that kinks on the screw dislocation are perfect edge segments. E-segments all have the same length h, the unit kink height, while S-segments can be of any length. In the present work we choose for the length of the smallest S-segment $a = b$, where $\mathbf{b} = \frac{1}{2}\langle 1\bar{1}0]$ is the