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Stacking fault based analysis of shear mechanisms at interfaces in lamellar TiAl alloys

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ABSTRACT

The interfaces in lamellar TiAl alloys have a strong influence on the strength and deformability of the microstructure. It is widely accepted that their number and spacing can be used to tune these properties. However, the results of molecular dynamics simulations of sliding at γ/γ interfaces in lamellar TiAl alloys presented here suggest that important factors, namely the sequence of different interface types as well as the orientation of in-plane directions with respect to the loading axis, have to be included into meso-scale models. Simulations of bicrystal shear show significant differences in the deformation behavior of the different interfaces, as well as pronounced in-plane anisotropy of the shear strength of the individual interfaces.

The critical stresses derived from bicrystal shear simulations are of the same order of magnitude as the one for nucleation and motion of twins in a γ-single crystal, showing that these mechanisms are competitive. In total four different deformation mechanisms, interface migration, twin nucleation and migration, dislocation nucleation, and rigid grain boundary sliding are observed. Their occurrence can be understood based on a multilayer generalized stacking fault energy analysis. This link between physical properties, geometry and deformation mechanism can provide guidelines for future alloy development.

1. Introduction

Recently developed TiAl alloys with lamellar microstructures, composed of the γ-TiAl and α_2-Ti_3 Al phases, show an enhanced ductility compared to the γ-TiAl single crystal [1–5]. However, further improvement in either the high or low temperature ductility is needed to make these materials useful for industrial applications. The challenge is to increase the deformability of the microstructure without lowering its creep resistance. To this end, the origins of ductility and the mechanisms of plasticity in the two-phase lamellar alloys have to be understood very well.

Nowadays it is clear that the interfaces in the microstructure play a crucial role for the plasticity, and that their number and spacing can be used to tune the deformability [5–10]. However, the exact influence of the interfaces on the deformation mechanisms is still unclear.

Conventionally, two main roles are assigned to the interfaces: presenting obstacles for dislocation and twin movement, and serving as dislocation sources [1,11]. Slip transfer phenomena through different interfaces in TiAl have been studied experimentally by Hu et al. [12] and for some specific cases by atomistic simulation by Katzarov et al. [13,14]. They demonstrate the effect of the misorientation of the slip planes, as well as of dissociation reactions that accompany slip transfer at different interfaces. The latter show the importance of the local atomic structure and associated energy barriers for slip within the interface plane. However, the atomistic simulations of Katzarov et al. [14] reveal two more effects: a significant reduction of Peierls stress for both ordinary and superdislocations when they lie in the interfacial boundary, and the stabilization of the planar core of superdislocations within lamellar boundaries due to the greatly reduced stacking fault energy at some interfaces. In other words the interfaces also influence the dislocation mobility within the lamellae. Furthermore, the cooperative action of dislocation motion and twinning inside the lamellae was suggested as the explanation [15,16] for the phenomenon of “channeled flow”, i.e. the phenomenon that under compressive load parallel to the interfaces the lamellar microstructure deforms only parallel to the grain boundaries, in a state of constant volume plane strain [17,18].

Experimental investigations of the effect of lamellar spacing on ductility, creep resistance and fracture toughness show that

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increasing the number of interfaces is energetically favorable [19], and enhances the ductility significantly [4,5,20] while actually increasing the creep resistance [5,21,22]. Thus decreasing the scale of a lamellar microstructure seems favourable, however, it raises the question if and when interface sliding based plasticity becomes important as an additional deformation mechanism. While some experimental studies report interface sliding and migration under creep conditions [9,23,24], others indicate that the deformation is accommodated wholly by dislocation based plasticity [5,21], even in very fine spaced lamellae.

In the paper at hand we investigate the intrinsic mechanisms of interfacial sliding in ideal bicrystals, i.e. without any dislocation or other further defects in the model. We carried out molecular dynamics simulations of shear at the three types of γ/γ interfaces along all possible directions within the interface planes. In total, four different shearing mechanisms were observed during dynamic loading. The strong orientation dependence of the mechanisms demonstrates the necessity to monitor the orientation of in-plane directions with respect to the applied load. The different mechanisms are interpreted and directly connected to SFE values and distributions at and around the interfaces. For this analysis we introduce a *multilayer generalized stacking fault energy* surface (multi-GSFE) calculation for the γ/γ interfaces. This quasistatic approach enables us as well to discuss the influence of the grain boundaries on possible dislocation dissociation reactions close to the interface and will be helpful for future atomistic studies.

The paper is organised in the following way. We explain our methodology in section 2, including details of the newly introduced, quasistatic, multilayer generalized stacking fault energy surface calculations, as well as of the molecular dynamics simulation of bicrystal shear. The results are presented in Section 3, starting with the multi-GSFE calculations, Section 3.1, which show a strong anisotropy of the energy landscapes for shear. In the molecular dynamics simulations we observe four main mechanisms along twelve different in-plane loading directions. We present one example for each mechanism in detail in Section 3.2. The anisotropy of the strength is discussed in Section 4.1 The understanding of the observed mechanisms based on the multi-GSFEs is developed in Section 4.2. In Section 4.3 we discuss the possible contributions of the different mechanisms to the overall deformation and compare our predictions with experimental observations. Final conclusions are drawn in section 5.

2. Methodology

2.1. Structure of γ/γ interfaces

Typical TiAl lamellar microstructures consist of many sharp γ/γ and a few α_2/γ interfaces which all are perpendicular to the $[111]\gamma$ and/or $[0001]\alpha_2$ directions. The crystal structure of the γ phase is $L1_0$, as shown in 1a. Different γ/γ variants can be created by rotating half of the initial supercell around the $[111]\gamma$ direction by 60°. Because of the tetragonality of the TiAl structure, there is a small mismatch between the <110> directions after rotation. Taking into account equivalent rotations, three different variants, the pseudo-twin (PT), obtained by 60° rotation, the rotational boundary (RB) by 120° rotation, and the true-twin (TT) by 180° rotation can be found, as shown in Fig. 1b.

2.2. EAM potential

For our simulations we used the ITAP molecular dynamics (IMD) code [25], and the embedded-atom method type interatomic potentials of Zope and Mishin for TiAl [26]. The potentials have been fitted to both experimental and first-principles data of various

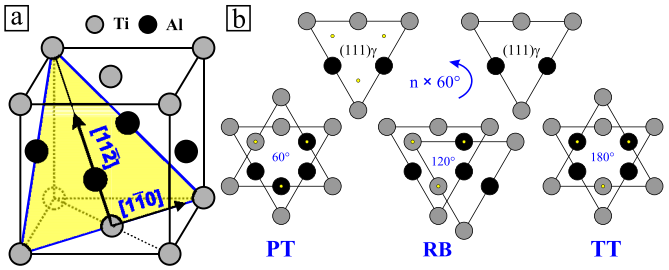

Fig. 1. a) $L1_0$ crystal structure of the γ phase, b) creating three different γ/γ interfaces by rotating the crystal structure around the [111] direction by n× 60°: the pseudo-twin (PT), obtained by 60° rotation, the rotational boundary (RB) by 120° rotation, and the true-twin (TT) by 180°.

crystal properties and structures in the Ti–Al system, and give a very good description of fundamental properties such as point defects and planar fault energies [26,27]. Nevertheless, among the known deficiencies of EAM potentials for this system is the fact that the anti-phase boundary (APB) in the single crystal is predicted to be metastable, in contrast to the results of DFT calculations, which show it to be unstable [28]. Indeed, our calculated GSFE surface of the γ-single crystal (111) plane (Fig. 2) exhibits a local minimum at the extension of the vector that marks the $[10\bar{1}]$ direction. However, it is very shallow, and otherwise this GSFE surface and generally those of the three γ/γ interfaces (see Section 3.1) are qualitatively and quantitatively comparable with the GSFE surfaces obtained from DFT calculations presented in Ref. [29]. Thus the results and discussions on the deformation mechanisms of the interfaces should not be affected.

2.3. Multilayer GSFE-surface (MGSFE) calculations

The conventional GSFE-surface calculation [30,31] is used to obtain the energy profile for shearing the single crystal parallel to the (111) plane. Half the supercell is shifted parallel to the shear plane (or mid plane of the respective single crystal supercell) and the atoms are allowed to relax perpendicular to the shear plane. The different shifts form a discrete mesh in the shear plane. The energy at each displacement is referred to the equilibrium structure,

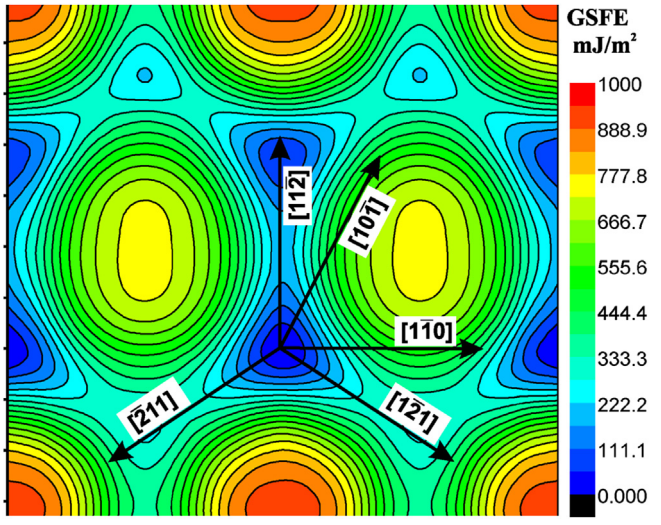

Fig. 2. GSFE-surface of the (111) plane of γ single crystal. The main shearing directions are indicated.