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Anisotropic shock response of titanium: Reorientation and transformation mechanisms

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Abstract

We investigate shock-induced phase transformations in titanium (α-Ti) single crystals induced by shock loading along the [0001], $[10\bar{1}0]$ and $[12\bar{1}0]$ directions using molecular dynamics simulations. We find a significant dependence of the microstructure evolution on the crystallographic shock direction, providing insight into the nature of the coupling between deformation and phase transformation. For shock along the *c*-axis, the orientation relationships (ORs) $(0001)_\alpha//(10\bar{1}0)_\omega$ and $[10\bar{1}0]_\alpha//[11\bar{2}3]_\omega$ between parent and product phases are observed, which differs from that previously reported for Ti. For shock compression along the $[10\bar{1}0]$ and $[12\bar{1}0]$ directions, there is a reorientation of the hexagonally close-packed α phase before the $\alpha \rightarrow \omega$ martensitic transformation, and the OR is consistent with the previously proposed Silcock relationship. We associate the reorientation with a shuffle and shear mechanism and suggest that shear stress is an underlying factor for the anisotropic phase transformation sensitivity.

Keywords: Shock compression; Martensitic transition; Titanium; Orientation relationships

1. Introduction

The group IV transition metal titanium (Ti) is amongst the most desirable of candidate materials due to its widespread and successful applications in the aerospace, nuclear and biomedical industries [1–4]. The allotropic phase transitions in pure Ti sensitively depend on tunable thermodynamic parameters such as external pressure and temperature. In particular, the pressure-induced martensitic hexagonally closed-packed (hcp) α to hexagonal ω transformation is important because ω phase formation affects toughness and ductility of Ti. This martensitic phase transformation can occur in α-Ti under hydrostatic, shock loading or high-pressure torsion conditions [5–7]. The room temperature (RT) $\alpha \rightarrow \omega$ phase transformation has been observed to occur at between 2 and 12 GPa, depending on the experimental technique, the pressure environment and the sample purity [8–12]. Furthermore, unlike the $\alpha \rightarrow \varepsilon$ transformation in pure Fe, the $\alpha \rightarrow \omega$ transformation in Ti exhibits a large hysteresis that is responsible for retention of the metastable high-pressure ω phase on release to atmospheric pressure [5,6,8].

Transmission electron microscopy (TEM) has been extensively used to understand the crystallography of the $\alpha \rightarrow \omega$ transformation. As this transformation is accompanied by hysteresis and can be irreversible, the high-pressure hexagonal ω phase can be retained partially or almost fully after unloading under ambient conditions [7]. Although this is well established under both static and shock conditions, the crystallographic nature of the transformation in Ti and Zr is still controversial [11,13–16]. In particular, it

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is not clear how the orientation relationships (ORs) depend on loading conditions. Moreover, little is understood about the coupling of deformation processes to phase transformation. Textural analysis below and above the phase transformation pressure suggests microstructural reorientation [11]; however, the nature of deformation twinning or dislocation slip mediating the transformation is not clear. Measurements to date have been primarily on polycrystalline samples and the anisotropy in shock response is not easily inferred from these measurements. Thus, our focus here is on studying the anisotropic response in single crystals, thereby providing insight into the factors mediating the phase transformation. We also suggest the types of measurements that can corroborate our findings.

ORs are key signatures of pathways that lead to a given microstructure. Essentially three ORs between the starting α and final ω phase have been observed so far in TEM studies of polycrystalline samples of Zr and Ti under different loading conditions. These are the so-called Variant I with the ORs $(0001)_\alpha//(10\bar{1}1)_\omega$ and $[10\bar{1}0]_\alpha//[\bar{1}011]_\omega$, Variant II with the ORs $(0001)_\alpha//(1\bar{2}10)_\omega$ and $[1\bar{2}10]_\alpha//[0001]_\omega$, and the form proposed by Song and Gray [14] or Variant III with the ORs $(0001)_\alpha//(10\bar{1}0)_\omega$ and $[10\bar{1}0]_\alpha//[11\bar{2}3]_\omega$. The first two were initially proposed by Usikov and Zilbershtein on the basis that the $\alpha \rightarrow \omega$ transformation occurs via an intermediate β phase [17]. Variant I has been primarily observed in hydrostatic and steady-state pressure conditions in both Zr and Ti in the pressure range 2.9–9 GPa at RT [14]. This OR was also later observed by Vohra et al. in dilute Ti–V alloys [18]. Variant II has been observed in pressure-treated Zr samples by Rabinkin et al. via electron diffraction measurements [19]. In pressure studies of Ti alloys, Silcock observed a direct $\alpha \rightarrow \omega$ transformation pathway for which the OR is the same as Variant II [20]. Note that although this OR is the same as Variant II, the pathways are quite distinct. Over the last few years, the availability of computing power has made feasible the enumeration of atomic pathways in crystals, especially for non group–subgroup transformations such as in Ti and Zr. Following this prescription, Trinkle et al. enumerated the lowest-energy pathways in Ti under hydrostatic pressure and discovered a direct pathway (TAO-1) with a lower energy than that noted by Silcock. This pathway has the same OR as Variant I [16]. Recently, there have been a number of studies involving high-pressure torsion (HPT) measurements on polycrystal Zr and Ti. The loading conditions favor shear-driven transformations leading to almost complete transformation to the ω phase. However, the mechanism has not been particularly well studied, although it has been suggested that the OR is consistent with TAO-1 [8]. There have been a number of studies of the ORs on shocked samples of Zr polycrystals. These studies largely find the same OR as Variant II [21]. The exception is the analysis by Song and Gray [14] who observed Variant III [11,14] and also proposed a specific pathway. This OR has been recently re-examined with the conclusion that it is a subset of Variant I [15].

Our objective here is to investigate how the ORs and transformation pathways are influenced if a Ti single crystal is shocked in different directions. Moreover, in order to explain the range of behavior seen in the above experiments, we study the effects on the phase transformation of the deformation behavior during shock compression and the anisotropy of the shock response. We find that loading along the *c*-axis gives rise to the ORs $(0001)_\alpha//(10\bar{1}0)_\omega$ and $[10\bar{1}0]_\alpha//[11\bar{2}3]_\omega$, which have not been observed previously though are related to the ORs seen in shocked polycrystal samples of Zr [14]. However, under shock compression along the *a*-axis, the α-Ti crystal experiences first an effective 90° rotation, which is induced by a shear and shuffle (or atomic displacement mode) mechanism. This is followed by the $\alpha \rightarrow \omega$ phase transformation. The OR is consistent with the Silcock relationship or Variant II, and the pathway is the same as Silcock. We suggest that shear is an underlying factor responsible for the anisotropic phase transformation sensitivity.

2. Computational method

The molecular dynamics (MD) simulations were carried out using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code [22] and a Ti modified embedded atom method (MEAM) potential with a cubic-splines-based functional form [23]. This potential removes the constraint of fixed angular character and allows for additional flexibility of the potential compared with traditional MEAM potentials. The EAM views each atom as embedded in a host lattice consisting of all other atoms. Each atom in the system is viewed as an impurity that is part of a host of all other atoms. The "embedding energy" of the impurity is determined by the electron density of the host before the impurity is added. The energy of an atom (or impurity) is represented as a two-body energetic interaction plus an embedding energy computed on the basis of an empirical electron density. Incorporating angular terms in the EAM density functional has led to the development of spline-based MEAM:

$$E_i = \frac{1}{2}\sum_j \phi(r_{ij}) + U(\rho_i), \tag{1}$$

with the density at atom I given by:

$$\rho_i = \sum_j \rho(r_{ij}) + \sum_{jk} f(r_{ij}) f(r_{ij}) g[\cos(\theta_{jik})], \tag{2}$$

where $\phi(r_{ij})$ is a direct two-body interaction between atoms i and j that depends only on the interatomic separation r_{ij}. The total effective electron density ρ_i at atomic site i contributes to the total system energy through the embedding function $U(\rho_i)$. The density $\rho(r_{ij})$ represents the contribution to the total effective electron density at atom i due to atom j a distance r_{ij} away. A radial cutoff function $f(r)$ and a three-body angular term $g(\cos(\theta))$ is used to describe