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Coupling between plasticity and phase transition of polycrystalline iron under shock compressions

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ABSTRACT

Coupling between plasticity and martensitic transformation is the origin of many properties of the material exhibiting martensitic phase transition, such as transition induced plasticity (TRIP) steels and shape memory alloys. Despite of great achievements made in the TRIP steels, studies to uncover the underlying coupling mechanism between plasticity and phase transition of iron under extreme pressures at lattice level are rarely seen. It is the underlying reasons for many mechanical behaviors of materials exhibiting martensitic transition under shock compressions. In this work, NEMD simulations are performed in polycrystalline iron under shock compressions with our recently developed interatomic potential which has been carefully validated for high pressure applications previously. With a lattice tracking algorithm specially designed for this study, orientation relationships between parent phase and transition product, and grain rotations are found out through texture analyses, both of which indicate more than one phase transition mechanisms emerge during the shock upon polycrystalline iron. Our results show that plasticity contributes to the phase transition of iron through two different coupling modes that resulting in two different phase transition mechanisms. Detailed scenarios of the two coupling modes, corresponding to the two phase transition mechanisms, are built in terms of infinitesimal slips among possible slip systems of α-iron. To clarify the difference of underlying natures of the two coupling modes, selection rules of martensitic variant, corresponding to the two modes, are found out, which agree well with our predictions.

1. Introduction

Martensitic phase transition of iron from α to ε phase, first discovered by Bancroft et al. (1956), is known to occur at large pressure, starting at 13 GPa and completing at around 23 GPa in shock compression experiments, which is of great interesting

List of abbreviations: ACNA, adaptive common neighbor analysis; DAC, diamond anvil cell; EAM, embedded-atom model; GB, grain boundary; LLTA, local lattice tracking algorithm; MD, molecular dynamics; NEMD, non-equilibrium molecular dynamics; ODF, orientation distribution functions; OR, orientation relationship; PDF, pole density function; SACM, stress assisted coupling mode; SAT, stress assisted transformation; SICM, strain induced coupling mode; SIT, strain induced transformation; SS, stainless steel; TP, transition pressure.

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among research communities due to its technical and scientific significance. Because of the transient and reversibility of this transition, it is not until recent decade that direct experimental observations of the phase transition under shock compressions are available (Kalantar et al., 2005; Wang et al., 2013; Yaakobi et al., 2005). Combined with non-equilibrium molecular dynamics (NEMD) simulations, phase transition mechanism has been well established for single crystalline iron under the shock along different crystallographic orientations (Hawreliak et al., 2006; Kadau et al., 2005; Wang et al., 2014a). The phase transition mechanism is believed to be the first one of previously proposed three possible mechanisms reviewed by these references (Pang et al., 2014b; Wang et al., 2014a), which is a two-step process. In the first step, atoms in $(110)_{BCC}$ plane will be compressed along $[001]_{BCC}$ axis (and slightly expand along $[\bar{1}10_{BCC}]$) to form a hexagon. The second step is a shuffle among alternate $(110)_{BCC}$ planes to establish a HCP lattice with its c axis lying along $[110]_{BCC}$. Although this transition mechanism could well explain the transition deformation and the orientation relationships (ORs) between parent phase (BCC) and transition products (HCP), it cannot predict detailed transformation scenario for preferred selections of the transition products (martensitic variants) which is of key importance for micromechanical behaviors of materials exhibiting martensitic transition (Cherkaoui et al., 2000; Li et al., 2014). It is well known that the phase transition is preceded by plasticity in experiments at nanosecond time scale. To achieve the phase transformation from α phase to ε phase, the preceding plasticity should accommodate to the phase transition mechanism, which will influence the selections of martensitic variants. However, few attentions are paid on the coupling behavior between the plasticity and the phase transition mechanism at lattice level. One of the reasons is due to a lack of interatomic potentials of iron appropriate to the high pressure condition. Commonly used interatomic potentials of iron can neither reproduce the preceding plasticity and phase transition simultaneously or avoid the emergence of a large fraction of artificial FCC phases under the shock upon polycrystalline iron (Kadau et al., 2007) or along high index crystallographic directions of single crystalline iron (Kadau et al., 2005). Fortunately, new faithful interatomic potentials of iron are available now, which could well overcome the problems mentioned above when applied to the shock upon single crystals (Wang et al., 2014a) and ramp-shock upon polycrystals (Gunkelmann et al., 2014).

The coupling between plasticity and martensitic transformation is widely discussed in explaining nucleation and growth of $\gamma \rightarrow \varepsilon \rightarrow \alpha'$ phase transition of austenitic stainless steel (SS) during tension deformation (Talonen and Hänninen, 2007; Venables, 1962). At present, there are two coupling modes proposed for the SS. One is believed to contribute to the phase transition through the nucleation of martensite at the generated dislocations and shear bands in the austenite (Talonen and Hänninen, 2007), which is referred to as strain induced transformation (SIT) in this work. Nucleation of the martensite could be regarded as generating a nucleus of certain kinds of lattice defects, whose driving force is written as

$$\Delta G_{SIT} = nV_0(\Delta G_c + \Delta G_s) + 2E_\sigma \tag{1}$$

where ΔG_c and ΔG_s are chemical free energy difference and strain energy per unit volume, respectively. The martensite contains n atoms with an average volume of V_0. E_σ is surface energy component of related lattice defects. Since the martensitic transformation completely couples with the plastic processes, the selection of the martensitic variants is governed by Schmid factor criterion. The other one contributes to the phase transition via a so-called stress assisted mode (Das et al., 2011) (referred to as stress assisted transformation or SAT), which is described in terms of a mechanical driving force ΔG_M adding to any chemical potential change due to the transformation

$$\Delta G_M = \sigma_N \delta + \tau s \tag{2}$$

where σ_N and τ are the normal and shear stresses resolved on the habit plane of martensite, and δ and s are the corresponding dilatational and shear strains accompanying the formation of the martensite. Compared with the formula (1), the lack of the surface energy in the (2) is because phase transition of this mode usually nucleates at preexisting defects. Analyses of a large amount of published data relating the fraction of martensites to plastic strain suggest that the SAT is more appropriate for interpreting experimental data than the SIT (Das et al., 2011). Moreover, most recent experiments conducted by Li and coworkers (Li et al., 2014) have shown that selections of martensitic variants obey minimum strain work criterion (Humbert et al., 2007) rather than Schmid factor criterion. Interestingly, the minimum strain work criterion satisfies minimum free energy condition under near equilibrium state according to the Formula (2), which indicates that the SAT is the underlying mechanism of the deformation induced transformation in the SS under the tensile deformation. However, the SIT could emerge in other experiments, for example the BCC-FCC phase transition of Molybdenum under the tensile loading (Wang et al., 2014b) and the $\alpha \rightarrow \varepsilon$ phase transition of iron using a rotational diamond anvil cell (DAC) (Ma et al., 2006). Systematic studies on these two modes of martensitic phase have been done by Valery I. Levitas (Levitas, 2004a, 2004b, 2004c) who found that the SIT requires completely different thermodynamics and kinetics treatment and experimental characterization comparing with the SAT. Further, micromechanical frameworks are developed for the two kinds of phase transition (Levitas and Ozsoy, 2009a, b; Levitas and Zarechnyy, 2010) and make a great success in interpreting the results of DAC experiments (Feng and Levitas, 2013; Zarechnyy et al., 2012). Despite of these achievements, studies to uncover the detailed coupling mechanism between plasticity and phase transition at lattice level are still lack, which is essential for the micromechanical models to improve their prediction capabilities. Furthermore, comparisons of the two modes at atomic scale are rarely seen, especially for the same phase transition. Besides, unlike FCC metals (such as the SS), dislocations in BCC metals are not easy to split due to its high stacking fault energy and its slip lines are wavy. The usual way of thermodynamic study of reconstructive