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An atomic study on the shock-induced plasticity and phase transition for iron-based single crystals

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ABSTRACT

The martensitic phase transition $\alpha \rightarrow \varepsilon$ of iron is of particular interest to researchers and industrialists due to its technological and scientific significance in recent decades. Experimental and numerical studies have discovered and confirmed the phase transition mechanisms under shock loading. However, the relation between plasticity and the phase transition, which is of key importance in understanding the material behavior under dynamic loading, has not been made clear, and former NEMD simulations fail to reproduce the plasticity observed in experiments. In this work, a new embedded-atom-model potential for iron has been developed and validated. Large-scale NEMD simulations are performed with a variety of loading strengths along three low index crystallographic directions, i.e., [001], [110] and [111], and the phase transition mechanism is examined with the aid of the *c* axis analysis technique proposed in this work. The differences in shock response to the different loading directions are explained by rotation symmetry and compression mechanisms as the first step toward phase transformation of iron. Although no well-defined plastic process is observed for the shock along the [100] and [111] directions, nucleation, propagation and multiplication of dislocations are clearly observed, and the slip system associated with plastic slip is determined to be $\{112\}\langle 111\rangle$ when loading along the [110] direction.

1. Introduction

The martensitic phase transition $\alpha \rightarrow \varepsilon$ of iron, which occurs at approximately 13 GPa, is of particular interest to researchers and industrialists, due to its technological and sociological significance in the development of human civilization, as well as its dominant role in the earth's core. The transformation is reversible and transient, which makes it very difficult to investigate. It is believed to contain richer details under shock loading than in static high-pressure environments, even for a single crystal (Branicio et al., 2013). With the great advance of computational capabilities and experimental techniques, we are enabled to study the material behaviors in response to dynamic compression deep into the lattice level (Lorenzana et al., 2008). Since Kalantar et al. (2005) first reported the direct observation of the $\alpha \rightarrow \varepsilon$ transition in shock-compressed iron via nanosecond X-ray diffraction and confirmed the phase transition mechanism proposed with non-equilibrium molecular dynamic (NEMD) simulations along the [001] direction (Kadau et al., 2002b), a series of experimental and numerical works

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have been devoted to uncovering the transition processes. Yaakobi et al. (2005) provided direct evidence of the phase transformation by extended X-ray absorption fine structure (EXAFS) measurements on polycrystalline iron shocked to 35 GPa. The orientation relations between the parent phase and the product phase, known as the Nishiyama–Wassermann relation, and whether the *Y* phase is emerged during the phase transformation are hotly debated issues. Kadau et al. (2005) found a large fraction of FCC phase under shock loading along the [1 1 0] and [1 1 1] crystallographic directions of single crystal iron by NEMD simulations. The orientation relationship of the parent and product phase are determined to be $\{1\,1\,0\}_{BCC}||\{0\,0\,0\,1\}_{HCP}$ and $[0\,0\,1]_{BCC}||[\bar{1}\,\bar{1}\,2\,0]_{HCP}$. Combined with non-equilibrium molecular dynamic (NEMD) simulations, three possible mechanisms of the $\alpha \rightarrow \varepsilon$ phase transition of iron have been proposed, and the first mechanism is confirmed by experiments when shocking along the [0 0 1] for iron single crystals (Kalantar et al., 2005; Hawreliak et al., 2006b). Mechanism I accomplishes a transition from the BCC lattice to a perfect HCP lattice through uniaxial compression along the $[0\,0\,1]_{BCC}$ direction by 18.4% to form a hexagon in the $(1\,1\,0)_{BCC}$ plane and then shuffling along alternate $(1\,1\,0)_{BCC}$ planes by $a/3\sqrt{2}$ (where a is the lattice parameter of initial BCC lattice) to establish an HCP lattice whose c axis lies along the $[1\,1\,0]_{BCC}$. Mechanism II is based on shear of the $(\bar{1}\,1\,2)_{BCC}$ planes along the $[\bar{1}\,1\,\bar{1}]_{BCC}$ direction, forcing atoms in the $(1\,1\,0)_{BCC}$ planes into hexagonal patterns, leading to a compression of 13.4% and a rotation of the lattice in the $(1\,1\,0)_{BCC}$ plane by 5°, followed by an additional shuffle process among alternate $(1\,1\,0)_{BCC}$ planes, as in Mechanism I. Mechanism III (or Mechanism IIa) is similar to the second mechanism in the first step. The only difference is a period-doubling process provided by the shuffle of alternate planes in the second step of Mechanism II. For Mechanism III, the second step is divided into two steps: the first is to form a metastable FCC phase and the second is to form a final HCP phase rather than directly forming the final HCP phase as in Mechanisms I and II. However, X-ray diffraction cannot distinguish the last two mechanisms because their final products are the same (Hawreliak et al., 2006a). Based on femtosecond laser driven shock synthesis of the high-pressure phase of iron, Sano et al. (2005) suggested that the *Y* phase could be induced as an intermediate structure between the $\alpha \rightarrow \varepsilon$ transition and explained this by the fact that a part of the FCC structure does not transform to the HCP structure when the additional pressure is insufficient or there is not enough waiting time. Kadau et al. (2007) showed that an experimental distinction between the HCP and FCC phases is not possible based on the EXAFS spectra alone, which is demonstrated further by Higginbotham et al. (2009). Hawreliak et al. (2011) performed *in situ* X-ray diffraction measurements of the c/a ratio in the high-pressure ε phase of shock-compressed polycrystalline iron and found no FCC phase as predicted by the NEMD simulations, which may be due to the difference in the time scale between their experiments and typical MD simulations, according to his explanation. Experiments conducted by Wang et al. (2013) found that the signature orientation relationships are consistent with phase transition Mechanism I, and the intermediate Y-iron can be excluded in the phase transition of shock-loaded iron. The results of density functional theory (DFT) calculations also give valuable insight into these issues. Caspersen et al. (2004) suggested that shear stresses have a significant influence on the $\alpha \rightarrow \varepsilon$ transformation, which explained the observed hysteresis in the transition pressure (TP). Dupé et al. (2013) shed light on the manner of the shuffle process in the phase transition mechanism, which is consecutive rather than simultaneous shuffle.

The plasticity of BCC metals (represented by tantalum) under shock compression has attracted great attention recently (Higginbotham et al., 2013; Ravelo et al., 2012, 2013) in comparison with the most studied FCC metals (such as copper). None of the studied metals exhibit a phase transition under the considered pressure ranges. Though significant progress has been made in understanding the phase transition processes in iron, many related problems remain unclear, such as how plasticity occurs, the relations between plasticity and the phase transition, and the role the FCC phase played in the phase transitions. Plate impact experiments (Jensen et al., 2006) show that stress relaxation was observed for the [1 1 0] and [2 1 0] orientations, but it was not observed for the [1 0 0] orientation and the polycrystalline sample. These particularities for the [1 1 0] orientation, most likely associated with special processes, have long been noticed, but the reasons still remain unclear. Subject to the restriction of the existing potentials of iron under high pressure conditions, plasticity is scarcely observed in former molecular dynamics simulations (Kadau et al., 2005; Kadau et al., 2007). Gunkelmann and his coworkers (Gunkelmann et al., 2012) compared the four most commonly used interatomic potentials of iron and employed them in the analyses of the response of polycrystalline α-iron under homogeneous uniaxial compression. Their studies show that these four potentials of iron are not good enough to describe the dislocations and phase transition pressure simultaneously. The role of the FCC phase in the phase transformation is still ambiguous. Notably, whether the FCC phase appears as an intermediate structure is essential to distinguishing the last two phase transition mechanisms mentioned above.

In the present work, a new modified analytic embedded-atom-model (MAEAM) potential of iron has been developed for high pressure applications. The interatomic potential will be introduced at the beginning of this work, and further validations of this potential will be described throughout the work. Large-scale non-equilibrium molecular dynamics simulations (NEMD) are performed with this potential. Plasticity and phase transition are reproduced in our dynamic results, which enables us to clarify the transition mechanisms of α iron when shocked along three low index crystallographic orientations and to determine the role the plastic process played before phase transition. With the help of the proposed c axis orientation analysis technique, the c axis orientations of the transition products (ε iron) can be directly connected to the orientations of the mother phase (α iron) and have shown good consistency with the mechanisms mentioned above. Moreover, the needle-type martensite phase can be observed after shocking along the [1 1 0] and [1 1 1] directions, which is similar to recently reported experimental results (Wang et al., 2013). The obtained results show that the shuffle processes involved in the last step of the phase transformation take place among a group of equivalent {1 1 0} planes that satisfy n-fold ($n = 1,3,4$) rotational symmetry with respect to the loading direction. Plasticity is found to play a special role in the phase transition for shocking along the [1 1 0] direction.