



# Atomistic studies of shock-induced phase transformations in single crystal iron with cylindrical nanopores



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## ABSTRACT

Non-equilibrium molecular-dynamic simulations with our modified analytic embedded-atom model potential were carried out on single crystalline iron of idealized cylindrical nanopores to study the effect of defect on shock response. The results showed that the shock response and phase transformation were influenced by cylindrical nanopores. Reflection wave, “hot spot” can be clearly observed under [001], [110] and [111] loading directions, and the nucleation and growth of dislocations appeared for the shock along [110] and [111] directions. The critical stress of phase transformation, the nucleation sites and martensitic variants were obviously influenced by the cylindrical nanopores. In addition, stress assisted transformation mechanisms and strain induced transformation mechanisms were discussed, and the kinetics of the variants which caused by the presence of cylindrical pores were studied.

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## 1. Introduction

The study of the mechanical and structural response behavior of solids under extreme high-pressure is important to understand geophysical, astronomical processes and technological application. Since iron is the main component of inner core of Earth and has been widely used in modern industry and defense, its high-pressure phase transition has been investigated extensively. The martensitic phase transition  $\alpha \rightarrow \epsilon$  of iron was first reported by Bancroft et al. in 1956 [1]. Shock pressure of the phase transformation of iron varies from 13 GPa to more than 30 GPa, depending on the stress states [2], strain rates [3,4] and the shear deformation of samples [5]. The mechanism of phase transition under high pressure has been a focus of interest for a long time. To date, three possible mechanisms of the  $\alpha \rightarrow \epsilon$  phase transition of iron have been proposed. The first mechanism is that the uniaxial compression along [001]<sub>BCC</sub> crystal direction make the atoms on (110)<sub>BCC</sub> crystal plane arrange into hexagon, then the shuffling along alternate (110)<sub>BCC</sub> planes transform the crystal into HCP structure with c axis lying along the [110]<sub>BCC</sub> direction [6,7]. The second mechanism is that, the shear of  $(\bar{1}12)$ <sub>BCC</sub> planes along the  $[\bar{1}1\bar{1}]$ <sub>BCC</sub> direction forces atoms in the (110)<sub>BCC</sub> planes into hexagonal patterns, then the relative shuffle between the (110)<sub>BCC</sub> crystal planes trans-

form the crystal into HCP structure [8]. The third mechanism is similar to the second one in the first step which forces atoms in the (110)<sub>BCC</sub> planes into hexagonal patterns, but then a metastable FCC phase appears before the final HCP phase forms [8].

Recently, the relationship between plasticity and  $\alpha \rightarrow \epsilon$  phase transition of iron has received extensive attention. The coupling between plasticity and martensitic transformation was widely discussed in the study of austenitic stainless steel, and two coupling modes, stress assisted coupling mode (SACM) and strain induced coupling mode (SICM), were proposed [9,10]. The two coupling modes correspond to two different phase transition mechanisms, namely, stress assisted transformation (SAT) and strain induced transformation (SIT) mechanisms in our work, respectively [11]. SIT contributes to the phase transition through the nucleation of martensite at the generated dislocation and shear bands [9], and the selection of martensitic variants of SIT meets Schmid factor criterion [11]. While SAT does not need the assist of new defects [12], and the selection of martensitic variants of SAT meets the strain work criterion [11].

It is noteworthy that, in real engineering materials, there are different kinds of defect inevitably or artificially, such as impurities, voids, dislocations and grain boundaries, and so forth. These preexisting defects are generally known as the original positions of phase transition nucleation or damage development, so the pre-existing defects may also affect phase transformation property of material under shock loading. Various types of defects have been

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extensively studied experimentally and theoretically [13–31] to discuss their influence on the properties of materials. And most of these works were focused on the shock response, such as shock-induced void collapse and melting, dislocation emission from nanovoid, plastic deformation, the nucleation, growth and coalescence of void and vacancy emission. Certainly, the influence of various types of defects of iron also has been reported [32–38]. For example, interplay of plasticity and phase transformation in shock wave propagation in polycrystalline iron was studied [34], the results demonstrated that the phase transformation is preceded by dislocation generation at the grain boundaries (GBs), plasticity is mostly given by the formation of dislocation loops. The work of Cui et al. [35] presented the microview as well as the wave profile analyses on the phase transformation of iron with a nanovoid to understand the role of defect under shock compression. In addition, Shao et al. [37] also studied the model of single crystalline iron with a nanovoid to detect the dynamics of shock-induced structural transition. What's more, the model of single crystalline iron with cylindrical nanopores under shock loading was studied [38]. However, up until now the micro-mechanism that how the cylindrical nanopores influences the phase transformation of iron is yet to be systematically clarified. Meanwhile, the study of such defect is meaningful because the material containing extended cylindrical pores can be used for the development of filters, detectors, cooling elements in nanoelectronics, etc.

With the rapid development of computer science and technology, molecular dynamics (MD) simulation allows us to explore the influences of defects on phase transformation at the atomistic level. In this paper, we introduced a nanoscale cylindrical pore with different pore diameter into a single crystalline iron. Using the molecular dynamics method with our modified analytic embedded-atom model (MAEAM) potential, the influences of the cylindrical nanopores on the structural transformations as well as kinetics of the phase transition under shock loading were investigated.

## 2. Modeling and simulation

The molecular dynamics code LAMMPS [39] and our MAEAM potential of iron were used in this work to perform the simulations. The potential function of iron, which provides a better description of both dislocation and phase transformation properties than previously employed potentials, has been detailed in Wang's paper [7] and well validated in high pressure applications on the study of single crystals [7,40] as well as polycrystals [11]. To investigate the effect of crystal orientation on shock response, we first constructed three perfect single crystalline iron samples, with the Cartesian ( $X, Y, Z$ ) axes corresponding to the  $([100], [010], [001])$ ,  $([\bar{1}10], [001], [110])$  and  $([1\bar{1}0], [11\bar{2}], [111])$  crystal directions, and their sizes are  $17.16 \times 17.16 \times 167.61$  nm,  $16.99 \times 16.88 \times 192.04$  nm and  $16.99 \times 16.82 \times 195.39$  nm, respectively. And then we set a cylindrical pore at the center of a perfect sample with the cylinder axis along with  $X$  axis by removing the atoms within a certain cylinder radius. In addition, in order to explore the effect of defect size on the transformation rate during phase transition of single crystalline iron with a cylindrical nanopore, four samples with different sized nanoscale cylindrical pore are studied for each shock loading direction, and their cylinder radius are about 1/10, 1/8, 1/6 and 1/5 of the length of the simulation box along  $Y$  axis, namely 3.43 nm, 4.58 nm, 5.72 nm and 6.86 nm in diameter for  $[001]$  loading direction, and 3.2 nm, 4.2 nm, 5.6 nm and 6.4 nm in diameter for both  $[110]$  and  $[111]$  loading directions. Periodical boundary conditions were applied to the  $X$  and  $Y$  directions. To equilibrate our model systems, we first applied an energy minimization using the conjugate gradient method, and then the samples were equilibrated in NPT

ensemble with temperature from 800 K to 10 K for 68 ps. Shock wave loading was applied along the  $Z$  direction by taking a few surface atomic layers at one end of the sample as a piston and pushing the piston inward at a certain velocity ( $v_p$ ). Different shocking pressures were generated by setting different piston velocity of 0.2, 0.3, 0.5, 0.6 and 0.8 km/s. The shock simulations were performed in an NVE ensemble. The motion equations of the atoms are integrated by the velocity Verlet algorithm with a time step of 0.4 fs and the run durations are up to about 40 ps, thus allowing for sufficient time for plasticity and transformed phase. The system was initially at a temperature of 10 K, this low temperature was chosen in order to minimize thermal noise and thus to facilitate the analysis of dislocation formation.

Samples were visualized using adaptive common-neighbor analysis (ACNA) [41] within OVITO [42]. The local atomic stress is defined as [43]

$$\sigma_{ij}(\vec{r}) = \frac{1}{\Omega} \left[ \sum_{\alpha} \frac{p_i^{\alpha} p_j^{\alpha}}{m} A^{\alpha}(\vec{r}) - \frac{1}{2} \sum_{\alpha \neq \beta} \frac{\partial V}{\partial r^{\alpha\beta}} \frac{r_i^{\alpha\beta} r_j^{\alpha\beta}}{r^{\alpha\beta}} I^{\alpha\beta}(\vec{r}) \right] \quad (1)$$

where  $A^{\alpha}(\vec{r})$  is 1 if atom  $\alpha$  lies within average volume  $\Omega$  centered on  $\vec{r}$  otherwise is 0. Function  $I^{\alpha\beta}(\vec{r})$  is the fraction length of bond  $\alpha\beta$  which lies within average volume and satisfies  $I^{\alpha\beta}(\vec{r}) = I^{\beta\alpha}(\vec{r})$ . The wave profiles are analyzed by uniformly dividing our simulation domain into many small bins (with a thickness of about 6 angstrom each) along  $Z$  direction, and the average values of atomic stress as well as velocity calculated statistically over these bins.

## 3. Results and discussion

### 3.1. Shock wave profile

Using large-scale molecular dynamics simulation, we investigated shock response of a model single crystalline iron with a cylindrical nanopore. Fig. 1 has shown the stress profiles and particle velocity profiles at five certain moments along three low index crystallographic orientations with a piston velocity of 0.5 km/s, revealing wave propagation during shock compression and subsequent release from the surface of cylindrical nanopores. Our results showed a few common features among the three directions, for example, multiple wave structure can be observed under the three loading directions. As one can see from Fig. 1(a), a reflected wave appeared after the right travelling wave arrive at the cylindrical nanopore at about 16 ps when shock along  $[001]$  direction, and the reflected wave of shock compression is a tensile wave. The flow stress suddenly fell to a lower stress states behind shock front but rose up to the full peak stress states at the cylindrical nanopore, and the particle velocity suddenly increases behind shock front due to reflected wave, which was similar to the situation of  $[110]$  and  $[111]$  loading directions. In all these three loading directions, multiple-wave-structure can be clearly observed, but is different from traditional pictures, which propose that the first wave is associated with an elastic deformation, the second is attributed to plastic deformations, and the last results from a certain type of phase transformation according to the time evolution. Taking the stress profile, particle velocity and atomic configurations at 20 ps (Fig. 1(a)) as an example, we can divide the wave profile into three parts, corresponding to three typical regimes as shown in Fig. 1(a). Region I located at the very beginning of the shock front where only elastic compression occurs. Region II was the phase transition regime. Region III is associated with elastic compression process. According to the theory of shock waves, when incident wave propagates to the free surface, the stress keeps zero. And in this work, the local stress in the stress profile gradually decreases as a result of the reflection wave which can

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