



Effects of pressure on structure and mechanical property in monatomic metallic glass



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ABSTRACT

In this work we studied the effects of pressure on the local structures and mechanical properties of pure iron metallic glasses based on molecular dynamics simulations. It is found that, at a quenching rate of 1×10^{13} K/s, glassy states are obtained for pressure not > 20 GPa and crystalline phases are obtained at 25 GPa. Voronoi analysis indicates that the local structure of glassy iron changes with pressure, and the degree of local fivefold symmetry in the quenched systems decreases as the pressure increases. Compression test results indicate a negative correlation between the pressure and the yield strength, with the strength of the glass obtained at 20 GPa being 0.56 GPa (or about 10%) lower than that at 0 GPa. This study sheds light on the understanding of pressure-induced changes of local structure and mechanical property of monatomic metallic glasses.

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1. Introduction

Metallic glasses (MGs), fabricated by quenching from high temperature melts can be considered as “frozen” liquids with no long-range structural order, [1,2], and most MGs possess improved mechanical, chemical, and magnetic properties [3–9] due to the lack of structural defects, such as dislocations and grain boundaries, as in their crystalline counterparts. Generally speaking, physical properties of alloys with given compositions are closely related to their structure, and hence many efforts have been made to tune the local structure and properties of MGs [10–13]. Recently, a series of studies have shown that high pressure (HP) has a great impact on the properties of MGs [14], glass forming ability (GFA) [15–17], and crystal nucleation and growth [18–20]. For example, Wang et al. [21] found that high pressure increases crystallization temperature and the GFA of $\text{Zr}_{46.75}\text{Ti}_{8.25}\text{Cu}_{7.5}\text{Ni}_{10}\text{Be}_{27.5}$.

Nevertheless, the effects of HP on local structures in the atomistic scale, especially during the dynamic supercooling process, are still far from being well understood. For example, some authors have reported that HP results in higher ideal icosahedra fraction and in turn higher GFA [16,22], while others have proposed a different tendency [23–25]. One possible reason for such debates lies in the difficulty in studying the structural evolution experimentally as the quenched liquid has a poor thermal stability against crystallization [26]. Direct measurement and observation of the movement of atoms and atomic clusters are also almost impossible in experiments. These difficulties render

molecular dynamics (MD) simulations a favorable alternative approach to study the supercooling dynamics in atomistic scale [27–29]. With enough accurate interatomic potential, simulations can be in good agreement with experiments [30–33].

In this work, we investigate the effect of pressure on local structures and mechanical properties of amorphous iron by means of MD simulations. Voronoi tessellation analyses indicate that, with increasing pressure, the local fivefold symmetry in amorphous iron decreases while fourfold and sixfold symmetries enhance accordingly. Such changes of local structures results in a decreased yield strength of amorphous iron.

2. Simulation methods

To study the effect of pressure on iron during rapid cooling, the classical MD code LAMMPS was used [34]. The initial configuration contains 8192 iron atoms in a cubic box with periodic boundary conditions in three directions. Embedded atom method (EAM) potentials developed by Mendelev et al., which is well consistent with experiments, were applied to describe the interactions among the iron atoms [33]. The NPT (constant number of particles, pressure and temperature) ensemble was used throughout the simulation.

Starting from a cubic atomic arrangement, the system was heated to 2500 K and equilibrated for 1 ns (with a time step of 1 fs) under pressures ranging from 0 to 25 GPa. Keeping the constant pressure, the liquid iron was quenched to 300 K at a cooling rate of 1×10^{13} K/s. Then, the applied pressures (5, 10, 15, and 20 GPa, respectively) were released and the system was relaxed for 2 ns at 300 K. The final atomic structures in the systems are characterized by the pair distribution function (PDF),

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coordination number (CN) analysis and Voronoi tessellation analysis [35]. After the formation of glassy models, compression tests were carried out at 300 K by shrinking the box size along x-axis at strain rate $1.0 \times 10^{10} \text{ s}^{-1}$. Similarly, periodic boundary conditions are imposed in three directions during the compression processes.

3. Results and discussion

3.1. Global structural information: pair distribution functions and coordination number

The PDF is widely used to reveal the structural characteristic of liquid, crystal and amorphous structures. Fig. 1(a) shows the PDF curves of iron at different temperature during the rapid cooling under 0 GPa. In the temperature range from 1500 K to 2000 K, the PDF curves exhibit a homogeneous atomic distribution indicating that the models are in the liquid state. The simulated PDF curves at 1820 K are in good agreement with the experimental one of liquid iron [33,36]. When the temperature is below 1000 K, a split can be seen in the second peak of the PDF curves, which is known as the characteristic of MGs.

Fig. 1(b) displays the PDF curves of iron at 300 K after quenching under different pressure (0–25 GPa). When the applied pressure is no >20 GPa, the final configurations are amorphous, as indicated by the split of the second PDF peaks. With the increase of pressure, both the first and the second peaks in the PDF of amorphous iron show an inward shift. Meanwhile, with the pressure increases, the height of the first peak in PDF curves increases while its width decreases. These results imply that high pressure decreases the nearest inter-atomic distance and increases the local order degree in the atomic packing simultaneously. When the pressure reaches 25 GPa, a crystalline phase with sharp PDF peaks is obtained.

Coordination number is the number of atoms that are in the nearest neighbor shell of a given atom. Fig. 2 represents the distribution of CN at 300 K formed under pressure ranging from 0 to 20 GPa, respectively. It is seen that >95% of atoms in the systems have a CN ranging from 12 to 15.

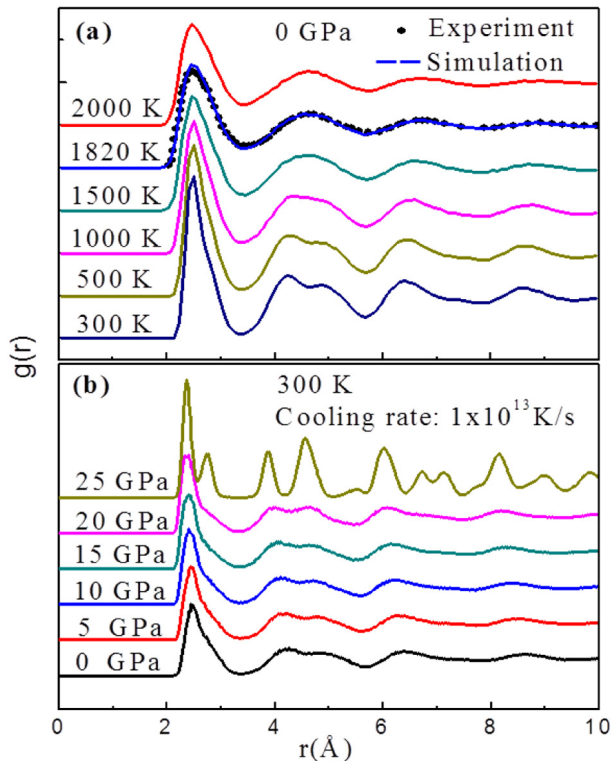


Fig. 1. Pair distribution function of iron (a) cooling under 0 GPa at different temperature and (b) at 300 K cooling under different pressure.

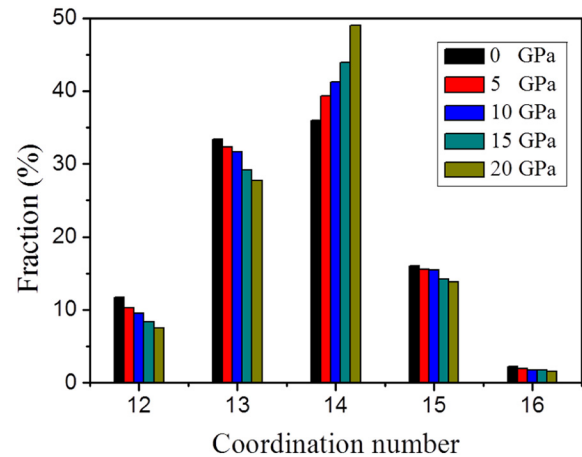


Fig. 2. Pressure dependence of coordination number distribution at 300 K.

The broad CN distribution indicates diverse local structures of the systems. Meanwhile, >35% the atoms have 14 nearest neighbors, which might be related to Frank-Kasper polyhedra. In addition, the fraction of atoms with 14-coordinated neighbors increases with pressure, while the fraction of atoms with other CN decreases. It is known that iron has a body-centered cubic (bcc) structure at room temperature, with atomic CN 14 [37]. The dominant and enhanced 14-coordinated clusters might be attributed to the enhancement of crystalline structural ordering, implying a tendency to crystallize with the increasing pressure.

3.2. Local structural information: Voronoi tessellation analysis

To further study the local structural difference of the amorphous models, we perform Voronoi tessellation analysis at 300 K. The Voronoi polyhedral index is expressed as $\langle n_3, n_4, n_5, n_6 \rangle$, where n_i donates the number of i -edged faces of the Voronoi polyhedron (VP).

Fig. 3 shows the ten dominant types of VP in different glasses under pressure from 0 to 20 GPa, and the inset shows the 3D distribution of atoms with VP $\langle 0, 6, 0, 8 \rangle$ in MD simulation cell at 20 GPa. It can be found that the fraction of each VP changed with pressure, indicating the changing of local atomic structures among the systems under different pressures although they all exhibit an amorphous-like PDF pattern. With the increasing pressure, particular attention should be paid to two types of VP: $\langle 0, 0, 12, 0 \rangle$, a kind of full icosahedron with complete

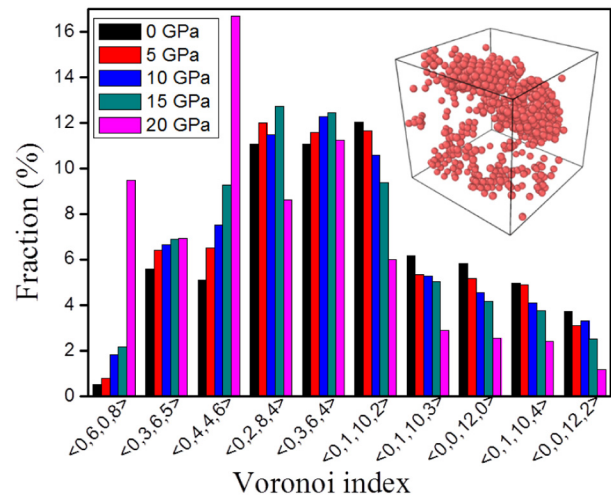


Fig. 3. Pressure dependence of dominated Voronoi polyhedrons in glassy iron at 300 K. The inset shows the distribution of polyhedron $\langle 0, 6, 0, 8 \rangle$ at 20 GPa.

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