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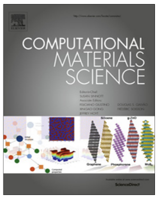

Effect of high pressure on the formation and evolution of clusters during the rapid solidification of zirconium melts

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ABSTRACT

The formation and evolution of clusters during the rapid solidification of liquid zirconium (Zr) under the pressure of 0–80 GPa were examined through molecular dynamics simulations. Local atomic structures were analyzed using pair-distribution function, Honeycutt–Anderson bond-pair index method, and developed cluster-type index method. Results revealed that Zr melts can be completely vitrified into a glassy state under 30–60 GPa. (13 1-1441 10-1551 2-1661) Kasper clusters, instead of (12 12-1551) icosahedra, dominate the formation of Zr metallic glasses. The numbers of Kasper clusters increase with increasing pressure. Under $\leq$20 GPa, the coexistence structures of the stable hexagonal close-packed (HCP) with meta-stable body-centered cubic (BCC) configurations are obtained with phase separation in the final solids. The fraction of BCC structures increases with increasing pressure. The evolution of basic clusters in the crystallization of Zr melts always takes the path of Kasper clusters → (14 6-1441 8-1661) BCC → (12 6-1421 6-1422) HCP. Crystallization under $\geq$70 GPa lacks an intermediate stage. Instead, the supercooled liquid (scl) Zr is directly transformed into A15 phase (scl → A15), which is composed of (12 12-1551) icosahedra and (14 12-1551 2-1661) Kasper clusters. The A15 structure is perfected with increasing pressure. Competition between densification and atomic diffusion contributes to the non-monotonic effect of high pressures on the rapid cooling of Zr melts.

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1. Introduction

A liquid-crystal (L-C) or liquid-glass (L-G) phase transition occurs when a metal is quenched from a liquid to a solid state. The appropriate conditions for the formation of metallic glass (MG), however, remain unknown [1,2]. Theoretically, all metal melts can be quenched into glassy states under a sufficiently high cooling rate, which suppresses the nucleation and growth of crystalline phases [3]. Nevertheless, only multi-component and limited binary alloys, such as Cu–Zr [4,5] and Pd–Si [6,7] can be experimentally formed into bulk MGs. Thus, the formation of MGs from pure metals remains challenging. Only a few monatomic MGs have been experimentally obtained through quenching the melts of pure refractory body-centered cubic (BCC) metals, including tantalum (Ta), tungsten (W), molybdenum (Mo), and vanadium (V), at an ultrahigh cooling rate of 10^{14} K/s [8]. The L-C or L-G pathway adopted by a metal during rapid cooling is intimately correlated with the local atomic structures of its melt [9–12]. Kasper polyhedrons [13,14], particularly icosahedra, have a critical role in the formation of multi-component MGs. Meanwhile, specific local atomic structures in melts likely exert strong effects on crystal nucleation and lead to the formation of a crystalline phase along the solidification path [15]. Therefore, investigating the evolution of the local atomic structures of metal melts during rapid cooling will help understand the microstructural origin of crystallization [16,17] and glass transition.

Pressure, an important thermodynamic parameter in addition to cooling rate [16], is a powerful tool for controlling and affecting vitrification and crystal nucleation during the quenching of metal melts [12,18] with the development of high-pressure techniques. Experiments have shown that high pressure remarkably affects the crystallization and glass transition of Zr- and Cu-based glassy alloys [19,20]. The constituent complexity of these multi-component alloys, however, hinders the investigation of the fundamental problems that concern microstructure transition in the rapid solidification of metallic melts [18,21]. Therefore, the effects of high pressure on the structural evolution of a simple model metal system should be systematically investigated. The transition-metal Zr is a good model metal system for exploring these fundamental problems given the excellent glass-forming ability of Zr-based glassy alloys with various compositions [1,19]

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and the pronounced increase in icosahedra in the supercooled liquid of pure metal Zr [22]. For example, Jakse et al. [23] have studied the short-range order (SRO) of liquid and undercooled metal Zr through ab initio MD simulation. Mo et al. [24] have very recently reported on the MD simulation of microstructural evolution in the crystallization of Zr melts that were rapidly supercooled at different cooling rates. However, to our knowledge, the effects of high pressure on local atomic structural transition in the rapid cooling of Zr melts have not been systematically investigated through experiments or computer simulations. Thus, in this work, we utilize MD simulations to study microstructural evolution during the rapid solidification of metal Zr melts under high pressure.

2. Simulation details

The rapid solidification processes of liquid metal Zr are simulated by adopting large-scale atomic/molecular massively parallel simulator (LAMMPS) code [25]. The simulation cell is a cubic box with three-dimensional periodic boundary conditions and contains 10,000 atoms that are initially arranged in an ideal HCP structure. The interatomic potential of metal Zr is the embedded-atom model (EAM) potential developed and shared by Sheng [26]. The EAM has been highly optimized through fitting potential-energy surfaces derived from high-precision first-principle calculations [24]. Our MD simulations are performed in an isothermal–isobaric (NPT) ensemble. The temperature is controlled using a Nose–Hoover thermostat [27]. The Andersen method [28] is applied to control pressure in every direction. The velocity–Verlet algorithm is used to integrate the motion equation with a time step of 1.0 fs. Zr is initially melted and equilibrated for 1 ns at 4000 K, which is well above the experimental melting temperature of T_m ~2127 K [22], under 0 GPa. Subsequently, the system is cooled down to 300 K at the cooling rate of 5×10^{11} K/s under pressures of 0, 10, 20, 30, 40, 50, 60, 70, and 80 GPa. The velocity and position of atoms and other necessary information about the systems are recorded per K for further analysis.

3. Results and discussions

3.1. Phase formation

Before the detailed microstructural analysis of the system, the evolution of the volume (V) per atom of metal Zr system with temperature (T) under various pressure levels is first analyzed, as illustrated in Fig. 1. The results showed that phase formation is strongly dependent on external pressure. Under 30–60 GPa, V did not abruptly change. This behavior suggests a glass transition event. By extrapolating and intersecting two linear parts in the V–T curve, the glass transition temperature T_g of the metal Zr rapidly solidified under 30, 40, 50, and 60 GPa is 623 K, 643 K, 715 K, and 735 K, respectively. Similar to the T_g of the $Ni_{50}Al_{50}$ alloy [12] and monatomic metallic Ta systems [29], that of the metal Zr increases with increasing pressure. Abrupt jumps within a narrow temperature range in the V–T curves are observed under 0, 10, 20, 70, and 80 GPa. This finding indicates that crystallization occurs in the quenching processes. The onset temperature of crystallization (T_c) is 1106 K (0 GPa), 1062 K (10 GPa), 862 K (20 GPa), 1016 K (70 GPa), and 1123 K (80 GPa). The end temperatures of crystallization (T_e) are 842 K, 802 K, 541 K, 554 K, and 1076 K. T_c and T_e decrease with the increase in pressure to ≤20 GPa. By contrast, pressures ≥70 GPa favor the increase in T_c and T_e. The opposing pressure dependence of T_c and T_e may be attributed to the differences in the microstructural evolution of the system during rapid solidification. Only one drop-off temperature emerges in the V–T curves obtained under 70 and 80 GPa, implying that a metastable phase is absent from the systems during crystallization. Unlike the volume contraction in other metal systems under ambient pressure, crystallization in the Zr metal system is associated with volume expansion under 10 and 20 GPa [1]. This interesting but expected observation could be well explained by the Clausius–Clapeyron relation (refer to Ref. [30]).

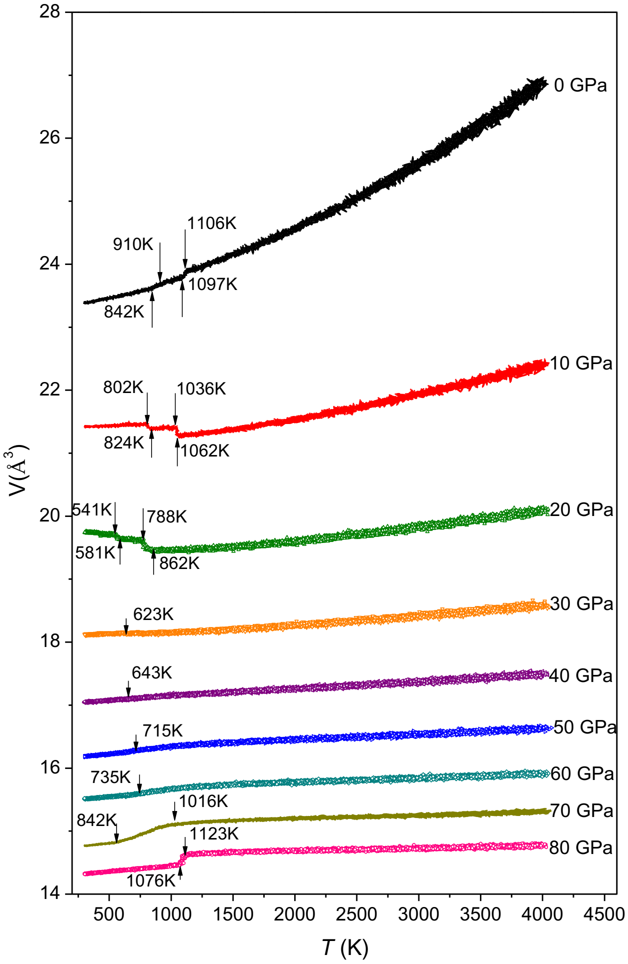

Fig. 1. The volume (V) per Zr atom in the system vs. temperature T in the processes of rapid cooling under various pressures.

3.2. Statistical analysis of microstructures

The pair-distribution function (PDF) is widely used to reveal the structural characteristic of crystal, liquid, and glassy structures [1]. The PDF g(r) is defined as follows: the mean volume V_n and the mean number of atoms N_n at a distance between r and $r + \Delta r$ from an atom are calculated over an interval of n time steps of the integration of the equations of motion. Then, g(r) is given by $g(r) = [N_n(r)V_n]/(4\pi r^2 \Delta r N)$.

Fig. 2(a) shows the comparison between the PDFs obtained through MD simulations and experiments under ambient pressure. The experimental results for the PDF at 1900 K are taken from Ref. [31]. The simulation results and previous experimental results are in excellent agreement. Our calculated $g(r)$ can be used to satisfactorily reproduce the experimental curve even for the second and third peaks. Fig. 2(b) further illustrates the PDF $g(r)$ curves of the final solids at 300 K under various pressures. Under 0, 10, and 20 GPa, the first peak of the PDFs is very sharp, and the second main peak splits into two sharp sub-peaks. This result indicates that the system is in a crystal state. However, under 30, 40, 50,

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