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Glass formation and cluster evolution in the rapidly solidified monatomic metallic liquid Ta under high pressure

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HIGHLIGHTS

- Pressure effect on glass formation and cluster evolution of Ta is simulated by MD.
- Defective icosahedra play a key role in forming Ta MGs.
- High pressure is unfavorable to form Ta monatomic MGs.
- GFA of liquid metal Ta can be estimated quantificationally by vitrification degree.

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ABSTRACT

Molecular dynamics (MD) simulations have been performed to examine the glass formation and cluster evolution during the rapid solidification of monatomic metallic liquid Ta under high pressure. The atomic structures in the systems are characterized by the radical distribution function (RDF), Honeycutt–Anderson (H–A) bond-type index method and cluster-type index method (CTIM). It is observed that the defective icosahedra play the critical role in the formation of Ta monatomic metallic glasses (MGs) rather than ⟨12 0 12 0⟩ perfect icosahedra, which have been identified as the basic local atomic units in many multi-component MGs. With the increase of pressure P, the fraction of icosahedral type clusters decreases remarkably in Ta MGs, while the fraction of bcc type clusters rises evidently. The evolution of vitrification degree (D_{SRO} or D_{MRO}) of the rapidly cooled metal Ta system further reveals that a higher pressure P is disadvantageous to the formation of Ta monatomic MGs. The weaker glass forming ability (GFA) of liquid metal Ta obtained under higher pressure P can be contributed to the decrease of D_{SRO} or D_{MRO} which is induced by increasing high pressure P to some extent.

1. Introduction

Although the first glassy metal was discovered over half a century ago [1], understanding the glass forming ability (GFA) of various metal systems remains a crucial issue in materials science [2]. Recently, many researchers have realized that GFA is intimately correlated with the local atomic structures of metal melts [3–6], especially the geometry and chemical composition of Frank–Kasper polyhedrons and their distorted cases [7]. Among them, icosahedral short-to-medium range orders have been demonstrated to play a critical role in forming a number of multicomponent MGs [2]. In the rapid

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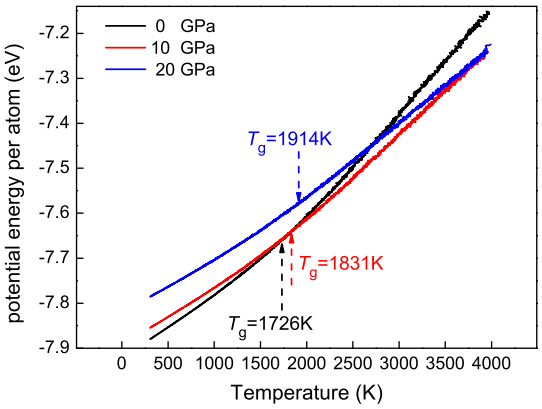

Fig. 1. The potential energy per atom as a function of temperature T in metal Ta system for various pressures P.

solidifying process, these icosahedral clusters exhibit a strong kinetic constraint for nucleation and growth of long-range crystalline orders [8], promoting the formation of metallic glasses. The constituent complexity for a multicomponent MG alloy, however, is not favorable to investigate the fundamental problems concerning the microstructures evolution and glass transition in the rapidly solidified processes of the metallic melts [9,10]. Therefore, it is highly desirable to carry out a systematic investigation on the glass formation and the evolution of local atomic structures in a simple model metal system.

As well known, it is a great challenge to make MGs for pure metallic liquids [9]. However, monatomic MGs have recently been successfully obtained in experiment by quenching melts of pure refractory body-centered cubic (bcc) metals, such as liquid tantalum (Ta) and vanadium (V), at an ultrahigh cooling rate of 10^{14} K/s [11]. The availability of monatomic MGs, being the simplest glass formers, offers unique possibilities for studying the GFA and the cluster evolution during the rapid solidification process [10,11] By *ab initio* molecular dynamics (AIMD) simulations atomic-level structures in Ta liquid and monatomic MG have been studied and the dominant polyhedra in Ta monatomic MGs are demonstrated to be the defective icosahedra rather than perfect icosahedra [10]. However, up to now, no fundamental understanding of the glass transition and local atomic structures evolution of these liquid metals under various quenching conditions exists. Thus, in present work, the glass formation and cluster evolution in the rapidly solidified processes of liquid metal Ta under various high pressures have been studied by MD simulations. The Honeycutt–Anderson (H–A) bond-type index method [12] and cluster-type index method (CTIM) [13–15] are applied to indicate the formations and evolutions of the local atomic structures. GFA of monatomic metallic liquid Ta and the competition of glassy orders with crystalline orders are further evaluated quantificationally by the vitrification degree D of the rapidly cooled metal Ta system.

2. Simulation details

With the help of LAMMPS code [16], a serial of molecular dynamics (MD) simulations of the rapid solidification processes of liquid metal Ta were carried out, in which 54 000 atoms in a cubic box subjected to the periodic boundary condition were considered, and their motion equations were solved by Verlet's algorithm in the velocity form with a time step of 1 fs. Constant pressure P and temperature T were imposed by the modified Nose–Hoover method [17] for both P and T variables and an embedded-atom model (EAM) potential developed recently for metal Ta [11] in a many-body framework was utilized. The metal Ta was initially melted and equilibrated for 10 ps at 4000 K well above the experimental melting temperature $T_m = 3290$ K [11], subsequently the liquid was cooled down to 300 K at the given cooling rate (5×10^{13} K s^{-1}) under different pressures ($P = 0$, 10 and 20 GPa). The cooling run was performed in the *NPT* ensemble with the given pressure. In present simulation, a primary temperature interval and the isothermal running time at selected temperatures were set as 50 K and 0.1 ps, respectively.

3. Results and discussions

3.1. Glass transition

Before analyzing the microstructures of the system in detail, the evolution of the potential energy (E_p) of simulated metal Ta system per atom as a function of temperature during cooling is firstly analyzed, as illustrated in Fig. 1. No abrupt change in E_p curves can be observed, indicating first order phase transitions such as the crystallization are absent [18]. By means of extrapolating and intersecting two linear parts of E_p *vs.* T curve from 300 to 3400 K, the glass transition temperature T_g of metal Ta is also deduced out. For $P = 0$ GPa, 10 GPa and 20 GPa, the evaluated T_g values are 1726 K, 1831 K and 1914 K, respectively. Present T_g values are in good agreement with other theoretical works [11]. Similarly to the result in Ref. [3], the present T_g ascends almost linearly with increasing P.