



Layering and phase transition of liquid aluminum confined by different substrates



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ABSTRACT

Molecular dynamics simulation has been performed to study the layering in the nano-confined liquid aluminum, a magic phenomenon characterized by oscillatory density profile across the molecular thin films. Carbon and copper walls are served as the confinement substrates, which can bring about discrepancy in the layering behavior, coordination number and diffusion coefficient. We highlight the abnormal changes of potential energy and volume when the new layer forms, accompanying the distinctive changes of the average coordination number and diffusion coefficient, which is a typical character of phase transition. The role of pressure and temperature on the layering is also reported. Specifically, the pressure-confinement and temperature-confinement diagrams are plotted to further analyze the layering transition.

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1. Introduction

The properties of material under confinement [1–10], which are distinct from those of the bulk, have received extraordinary research efforts due to their fundamental significance in both science and engineering. Examples include phase transitions, where the confinement can bring about the temperature shift of the freezing, melting and glass phase transition points [11–16]; self-assembly, where the confinement have its unprecedented potential in the area of device fabrications, thus precisely regulating internal structures of the target materials at the mesoscopic, nanoscopic and molecular levels [17–20]; and chemical reactions, where the confinement within carbon nanotubes enables the control of catalyst activity, morphology and stability [1]. Owing to a myriad of practical applications, investigations on properties of materials within confined space become remarkably significant.

The layering, a magic phenomenon under confinement, has been reported in terms of its non-uniform system density across the molecular thin films by Persson et al. [21]. Subsequent researches support the picture that the layering plays a key role in a multitude of fields. For instance, the layering of water molecules surrounding metal nanoparticle can lead to a greater thermal conductivity, thus increasing the heat transfer efficiency of the fluid [22]. The layering of alternating anions and cations in ionic liquid [23–26] is highly correlated with lubrication and catalysis.

Furthermore, the layering of hydrogen isotopes in the inner surface of carbon nanotubes can be applied for the separation of hydrogen isotopes [27]. Even in the dentistry, the layering techniques can be employed to achieve aesthetic purpose [28]. Considering the general significance and wide application, it is surprising that some details of the layering are poorly understood.

Another interesting problem is the mechanism of the layering transition, about which a considerable number of substances were reported. A first order phase transition [29] occurred involving the transformation between a bi-layer liquid and a tri-layer heterogeneous fluid in the confined water. Besides water [30–36], Saslow et al. [37] studied the Helium films with respect to its mono-layer to bi-layer transition using a Maxwell construction. In addition, layering transitions in the confined carbon [38], silicon [39], and silicon carbide [40] liquid films were also clarified with a noticeable structure change. Although remarkable advances have been made, the proofs of the layering transition are still limited especially in some liquid metals. Aluminum (Al) and its alloys are perceived as the most versatile and acceptable engineering materials which are widely used in aerospace components, automobile components and electrical appliances [41,42]. In present work, we confine the liquid Al between two parallel walls and observe its layering transition controlled by slit sizes (SS) and pressure. This simulation results can give insight into the properties of the liquid metal under confinement.

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2. Models and methods

MD simulations [43–45] are performed using the software package LAMMPS to study the structure of the liquid Al confined by carbon and copper walls. The interactions between the carbon walls and the liquid Al, which is initially arranged into $15 \times 15 \times 2$ face-centered cubic (FCC) lattice, are represented by 6–12 Lennard-Jones (LJ) potentials with the following parameters: ϵ_{Al}^- wall = 0.038 eV, σ_{Al}^- wall = 2.96 Å [46]. It is well known that the simulation results are highly dependent on the adopted potential functions and the previous studies mainly adopt Lennard-Jones potential as the carbon walls. In this study, the copper walls, whose interaction with the liquid Al is embedded-atom method (EAM), are also employed, where 2403 Al atoms are used. The pair interaction between metal particles is modeled with the EAM which is particularly appropriate for metallic systems.

Simulations are carried out using the NPT ensemble. The Nose-Hoover thermostat and barostat are adopted to control temperature and pressure, respectively, and the velocity-verlet algorithm is applied to integrate the equations of motion with a time step of 1 fs. The constant pressure parallel to walls (P_{xy}) is exerted to analyze the effect of pressure on the layering. Periodic boundary conditions are applied along the x and y directions. Along the z direction, the confined wall is imposed with the SS varying from 11 Å to 18 Å.

The liquid Al is equilibrated to obtain a relatively homogeneous liquid at high temperature of 2000 K. Then it is cooled to the target temperature (1300 K or 1200 K) at the cooling rate of 1 K/ps. Subsequently, the metal Al is relaxed at the target temperature for 2000 ps, which is adequate for the system to reach its equilibrium.

3. Results and discussions

Fig. 1(a) and (b) shows the density distribution function, which is calculated by counting the atom number in a thin slice with the thickness of 0.05 Å in the z direction, and the corresponding structure snapshots for the liquid Al confined by LJ interaction carbon

walls at 1200 K and copper walls at 1300 K respectively. Each density peak corresponds to an atom layer in the confined liquid as shown by dashed lines. The confined atoms aggregate at three or four density peaks, displaying an outstanding discontinuous distribution, contrary to the conventional wisdom that atoms can scatter uniformly in a free space. From Fig. 1(b), we can see that the density peaks adjacent to the confined walls are higher due to the stronger confinement effect, indicating that the confinement is essential for the layering. The density value of the liquid Al confined by copper walls (Fig. 1(b)) is larger than that confined by the carbon walls, suggesting the confinement effect of copper walls is stronger.

The alteration of SS can lead to the change of layer numbers as displayed in Fig. 2. For the liquid Al confined by carbon walls (Fig. 2(a)), the system keeps tri-layer structure at the SS range from 11 to 12.5 Å, which is named as the tri-layer zone. When the SS increases, the system starts to transform from three to four layers. Upon the SS increasing to 13 Å, the system totally transforms to four layers. Therefore, the SS interval from 12.5 to 13 Å is defined as the transition zone (TZ). The rest may be deduced by analogy, such as the transformation from four to five layers. However, when the liquid Al is confined by copper walls (Fig. 2(b)), the system transforms from four to five layers directly at the SS of 12.5 Å. As a result, the TZ disappears. Besides, the layer number is different under different slits with the same SS. For example, when the SS is 14 Å, the system shows tetra-layer and penta-layer structures for carbon and copper substrates respectively because the confinement extent is different. The system potential energy and volume as a function of SS are also displayed in Fig. 2. It can be found from Fig. 2(a) that at 1200 K, when the SS increases from 11 to 12.3 Å, the potential energy shows no big change. However, a sudden drop of the system potential takes place at the TZ, indicating the occurrence of the layering transition. A steady period of the potential energy at the tetra-layer zone is subsequently followed by another drop, where another layering transition also takes place. Fig. 2(a) also shows the system volume as a function of SS. It is instinctively understandable that the system volume would increase upon the

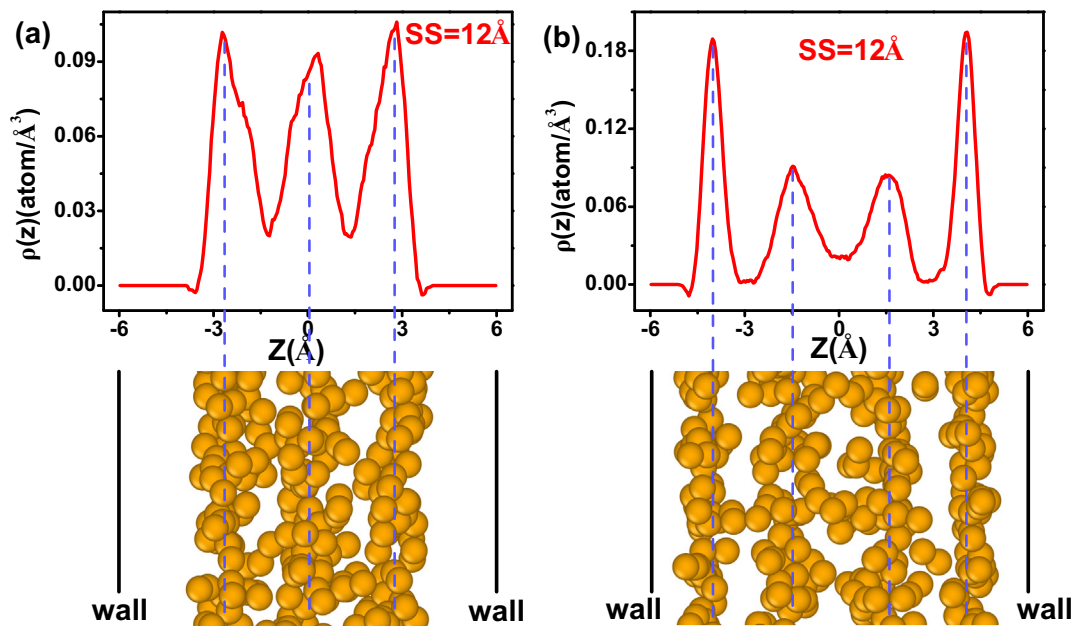


Fig. 1. Density distribution functions (ρ) and snapshots along the z direction of the Al atoms (a) confined by carbon walls when $T = 1200$ K, $P_{xy} = 0$ bars (P_{xy} refers to the lateral pressure along x and y direction), $SS = 12$ Å; (b) confined by copper walls when $T = 1300$ K, $P_{xy} = 0$ bars, $SS = 12$ Å. The confining walls are located at $z = -6$ Å and $z = 6$ Å as displayed by the solid black lines. The peaks in density profiles correspond to the layer locations in the snapshots, which are marked by dashed line. The system exhibits tri-layer and tetra-layer structure in (a) and (b) respectively.

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