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Full Length Article

Effect of curved surfaces on the impacting nano-droplets and their shape control: A molecular dynamics simulation study

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ABSTRACT

Considerable non-flat solid substrates are widely-existed where liquid drops inevitably impact on their surfaces, precise control of shape evolution of these impacting drops on such surfaces is desired in nature and some advanced technologies. Herein, a common but less-concerned substrate with curvature is used to investigate the impact dynamic of liquid metals by performing molecular dynamics (MD) simulations, which exhibits anisotropic impact behavior with distinct spreading and retraction in the two perpendicular directions and results in an elongated strip-like shape during shape evolution. The effects of curvature diameter, liquid properties (drop size and surface tension), and impact velocity are deeply demonstrated by quantitatively comparing the value of length ratio that is defined to describe the drop asymmetrical impact behaviors. This work helps advance our understanding of how the liquid metal evolves after impact on the curved surface and provides some feasible strategies to control its deposition and shape for some potential applications, such as 3D printing techniques, special coating, as well as drop-casting process.

1. Introduction

Drop impinging on solid surfaces is a central element of a wide variety of phenomena encountered in many technological applications, such as spray coating, inkjet printing, pesticide splashing, fire suppression by sprinklers, internal combustion engines, and criminal forensics [1], as well as in development of non-wettable or fully wettable surfaces for dropwise heat removal, anti-icing and water harvesting [2–7]. Therefore, understanding and controlling of the drop impact process have been a valuable research in both experimental investigation and theoretical modeling for recent years [8–21]. In addition, due to the large liquid-substrate interaction generated by the impingement force, study of the drop impact dynamics may develop new way to link the fluid properties and liquid-solid interfacial properties. It is well known that most impact dynamic can be divided into different stages, including spreading, retraction, deposition or rebound. Research has demonstrated that the spreading and retraction dynamics of impacting drops highly depend on the properties of liquid drop (such as surface tension, viscosity, density, and so on), the properties of underlying substrate (wettability and roughness) and the impact velocity [1,4,8,22–24]. However, it is worth noting that tuning the topography of the solid surface plays a dominating role in controlling the impact behaviors. Actually, the solid surface is usually rough and non-planar in reality, such as nanometer ridges [8], big conical posts [15] or chemical defects [25]. Therefore, the exploration of impact dynamic of the metal drop on a special or well-designed substrate becomes more attractive.

Recently, a great deal of improvement has been made in the study of drop impact on the superhydrophobic substrate [4,6–8,13,24,26,27]. By converting the surface energy into the kinetic energy, the impact drop can shrink and finally leave the substrate [28–30], which is known as the rebound or bouncing behavior. On the superhydrophobic surface, the specific function such as anti-icing, anti-fogging, self-cleaning and liquid recomposition can be achieved. Additionally, people also focuses on the slippery [12] or inclined surface [15,31,32] in the study of drop impact dynamics. Yeong et al. [31] investigated the drop oblique impact characteristics with a substantive range of Weber and Ohsnesorge numbers on the inclined substrate, and pointed out that the spread and rebound behaviors do not match the normal impact results on the equivalent flat substrates in most cases, which testifies the significant effect of the substrate morphology on the impact dynamics. In nature, most surfaces are usually convex or concave with some curvature, especially at the nanoscale, as exampled by the curved plant leaves with the countless nanofibers. Therefore, the drop impact on the curved surface attracts more and more interests. Liu et al. [23] designed an asymmetric convex surface with macrotextures and studied the impact behavior of water drop. Their experiment results showed that the bouncing dynamic has distinct spreading and retraction along the two perpendicular directions, leading to an asymmetric momentum and

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mass distribution that allow for preferential fluid pumping around the drop rim, which is revealed by their subsequent simulation research. However, the analysis and understanding of the detailed physical mechanisms about this impact dynamics are severely limited, especially for the liquid metal.

Until now, little work has been carried out on the impact dynamics of molten metals because of requirement of complex experiment device and difficulty in controlling liquid at room temperature. However, the impact behavior is a common process in the metallurgy when the metal drop splashes [33,34], and the study of the normal impact of liquid metals is important for a wide variety of industrial processes and applications, including electronic fabrication [35], thin film coating, and heat conductor production [36]. Typically, the shape evolution of the droplet after impact is significant to the materials formation, and thereby has a great influence on the materials properties. Hence, we carry out the molecular dynamics simulations to study the impact dynamics of liquid metals on the curved surface, which may provide theoretical guidance for controlling the impact dynamic of nano-sized metal drop.

2. Models and methods

Since the liquid metals are difficult to be operated in real experiment conditions, molecular dynamics (MD) simulations are performed to study the impact dynamics of liquid metal drops on the curved surface. Different diameters of carbon nanotubes (CNTs) with 135.60, 122.04, 108.48, 94.92, and 81.36 Å, are used as the curved substrates, where the inner and outer surfaces of the nanotubes can represent the convex and concave surfaces, respectively. Because we mainly investigate the effect of curved surface on drop impact dynamics, the CNT substrate is fixed to simulate the solid substrate and the chemical reactions can be ignored. This simplified model is helpful for improving the computational efficiency and eliminating the bad effects of other influencing factors. As such, the drops could neither penetrate nor deform the single-layer carbon substrate even under a big impact velocity. The liquid metal drops (D_0 = 50 Å) are initially deposited at a distance of 100 Å above the substrate as displayed in Fig. 1(a), and then released with a constant velocity to impact the curved surface. Also, the reaction between the high-temperature metal drops and the carbon nanotube substrates can be neglected because we mainly focus on the effect of curved surface on the drop impact dynamics.

The empirical many-body potentials of Al–Pb system have been constructed by using the "force matching" method, and are used for computer simulations of the Al–Pb system over a wide temperature range from 0 to 2000 K, which are fitted to experimental data and physical quantities [37]. Therefore, we here model the Al-Al and Pb-Pb interactions by the embedded atom method (EAM) potential, which can be written as: $E_i = F_\alpha(\sum_{j\neq i}\rho_\beta(r_{ij})) + \frac{1}{2}\sum_{j\neq i}\phi_{\alpha\beta}(r_{ij})$, where F is the embedding energy, φ is a pair potential interaction. For the C-C interaction, the adaptive intermolecular reactive empirical bond order (AIREBO) potential [38–40] is adopted. Due to the fact that metal and carbon can only form soft bonds via the charge transfer from the π electrons in the sp^2 hybridized carbon to the empty 4s states of metal [41], we use the 12-6 Lennard-Jones (L-J) potential to describe the Al-C and Pb-C interactions, which is expressed as: $E = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] r < r_c$, where ε is the depth of the potential wall, σ is the finite distance at which the inter-particle potential is zero, r_c is the cutoff with a distance of 10 Å, and the LJ parameters are: ε_{Al} = 0.0309 eV, σ_{Al} = 3.422 Å [42]; ε_{Pb} = 0.01751 eV, σ_{Pb} = 3.288 Å [43–45]. With these parameters, a basic test is carried out to valid our simulations. As shown in Fig. 1(b). we calculate the equilibrium contact angles of Al (83.43°) and Pb (112.12°) on the flat graphene at 1500 K, which accord well with the experimentally measured contact angle of Al (about 85°) [46] and Pb (about 110°) [47]. Thus, the simulation results based on carbon-metal system are reasonable and reliable.

The MD simulations are carried out using the large-scale atomic/molecular massively parallel simulator (LAMMPS) package in the NVT ensemble. The temperature is held at 1500 K which is controlled by the Nose–Hoover thermostat [48,49]. The time integration of Newton's equation of motion is calculated by the velocity verlet algorithm [50] with a time step of 1.0 fs. All MD simulations run for 300 ps to study the impact process.

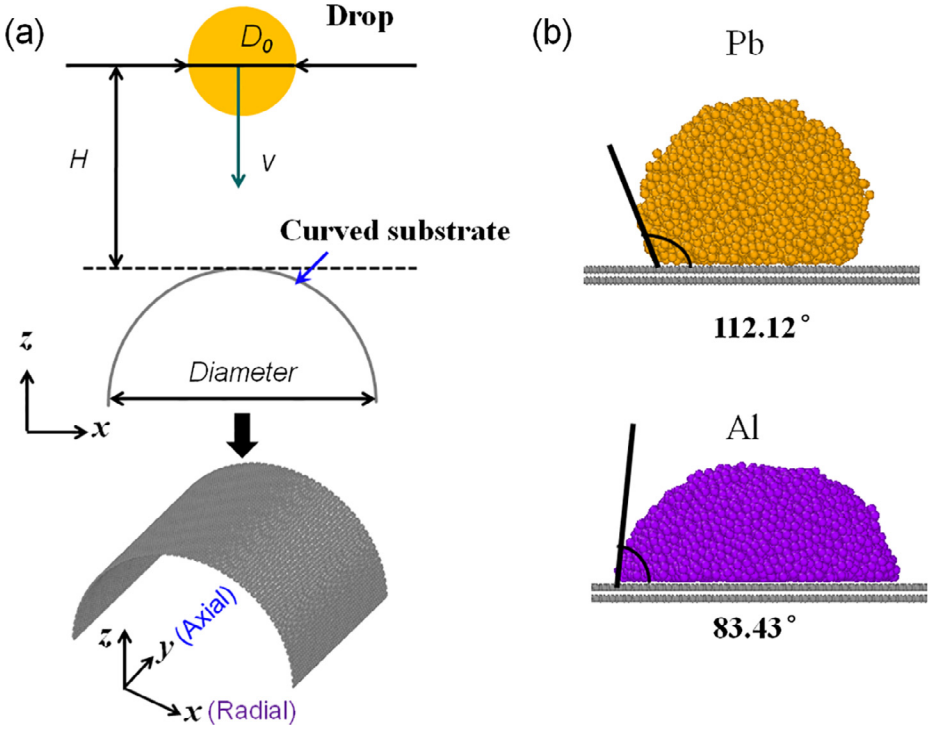

Fig. 1. (a) Schematic illustration of the models for our simulations, the top one is the side-view of the location of the impacting drop and the substrate, the bottom one is the full-view of the curved substrate (half of the carbon nanotubes), in which the x and y directions correspond to the radial and axial direction, respectively. (b) The equilibrium contact angles of Pb and Al on flat graphene at 1500 K.