



# Wetting characteristics of lithium droplet on iron surfaces in atomic scale: A molecular dynamics simulation

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## ABSTRACT

The wetting characteristics of lithium droplet on different iron surfaces are investigated in details by using molecular dynamics simulations associated with the modified analytic embedded atom model potential. In addition to the wettability of Li droplet on Fe (1 0 0), (1 1 0) and (1 1 2) surfaces, the wetting behavior on a polycrystalline Fe surface is studied. The results show that liquid Li can perfectly wets Fe surfaces, and the wetting behavior of Li droplet is isotropic on Fe (1 0 0) and (1 1 0) surfaces, but anisotropic on Fe (1 1 2) and polycrystalline Fe surfaces. For the Fe (1 1 2) surface, the anisotropic wetting is attributed to the lower energy barriers of Li atom diffusion along the  $[1\ 1\ \bar{1}]$  orientation on the Fe (1 1 2) surface. We have proposed a new method for describing the wetting behavior of liquid on substrates in atomic scale by measuring the time-dependent 'contact atom number'. The unified description of the liquid wetting on both single crystal and polycrystalline surfaces is achieved by this method. Li droplet wetting on the Fe (1 1 0) has the fastest spreading rate, and the spreading rate on the polycrystalline Fe surface is only faster than that on the Fe (1 0 0) surface. In addition, the effect of temperature on the wettability is examined, and it is found that the faster spreading occurred with increasing temperature.

## 1. Introduction

The liquid flow mechanism and phase change characteristics on solid surface are deeply influenced by the surface wettability, which plays a significant role in natural science, engineering technology and various industrial applications, such as coating, printing [1], mineral flotation, oil-based mud formula [2], lubrication, agricultural sprays and soldering [3–5]. A large number of experimental and simulation studies on wettability have been conducted to explore the wetting mechanisms, and the related achievements were summarized in Gennes' review article [6]. Some effective ways are proposed to improve the wetting properties, for instance, grooving and changing the chemical properties of solid substrate [7,8]. With a lattice-Boltzmann method, Fabiano et al. have simulated the wetting properties of liquid-vapor system [9]. Yin et al. have studied the dissolutive wetting behavior of Bi-Sn alloys on pure Bi substrates at 250 °C and found that the macroscopic contact angle is close to 90° during the spreading [10]. Molecular dynamics (MD) simulation is a helpful tool to investigate the wetting mechanism [11,12]. Huang et al. [13,14] have studied the

dynamics of metals clusters on a graphite surface using MD simulations with Lennard-Jones (LJ) potential. They confirmed that the wetting of metals on graphite can be well described by LJ potentials. Webb III et al. [15] have simulated the wetting of Pb on Cu (1 0 0) and (1 1 1) surfaces, and they found the precursor film spreading more faster on Cu (1 1 1) surface than on Cu (1 0 0) surface. Moon et al. [11] have studied the wetting of Ag on Ni (1 0 0) substrates, and the precursor film was formed during the wetting process. Webb III et al. [16] have investigated the wetting of eutectic AgCu system with MD simulations, and found that with the increasing proportion of Cu in the Ag-Cu droplet the spreading rate of the droplet on Cu surface decreased and an Ag-rich monolayer of atoms film did not appear until the dissolution was completed. Although the wettability of liquid droplet on substrate has been extensively simulated, most of them are performed on single crystal substrates, and less attention has been paid to the wettability of polycrystalline surfaces. However, the macroscopic experiments of wetting are generally performed on polycrystalline substrates. For further understanding the wettability of liquid on solid substrate, the exploration of droplet wetting on polycrystalline is necessary.

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In experimental and simulation studies, two common methods are used to characterize wettability from a macroscopic perspective. The contact angle ( $\theta$ ), which is defined as the angle between the tangent of liquid droplet at the contact point of a 3-phase (solid/liquid/gas) and the baseline of a solid substrate, has been widely used to characterize wettability [15,17–19]. To obtain the contact angle  $\theta$ , the key is to record the shape of Li droplet versus time  $t$  and locate the edge of Li droplet at different moments [20,21]. Another common method is measuring the time-dependent radius of the precursor film [15,16,22]. However, these two methods are not suitable to characterize the wettability of liquid on polycrystalline substrate. To this end, we proposed a new method to solve this problem, which will be introduced in the following.

Liquid lithium (Li), as a promising material of Plasma Facing Components (PFCs) for fusion devices, has been getting increased attention in recent years [23,24]. Liquid Li has an excellent particle pumping performance and has been successfully applied to many PFCs devices, compared with traditional materials [25–27]. The wetting property of liquid Li on the surface of structural material is a key issue for applying liquid Li limiter/divertor in fusion devices. Flowing liquid Li limiters (FLL) have been applied in HT-7 fusion device, [28,29], and the encouraging achievements demonstrate that investigating the wettability of Li on PFCs is a necessary work. The wetting behavior of liquid Li on select fusion-relevant surfaces (Mo, 316 SS etc.) have been studied by Fiflis et al. [30]. Surface pretreatment technologies, such as the pre-evaporated lithium layer and plasma cleaning via an argon glow method, are proposed very effective to reduce the wetting temperature of Li droplet on these surfaces. The wetting properties of liquid Li on Li compounds have been examined by Krat et al. [31], and they found that the liquid Li wettability on  $\text{Li}_2\text{O}$  and  $\text{Li}_3\text{N}$  surfaces were better than on fusion-relevant materials (W, Ta, and so on). The wetting of Li droplet on single crystal W and Cu surfaces have been studied with MD simulation by our group, the dewetting phenomenon of Li film from W surface is founded and the anisotropic wetting appears on the Cu (1 1 0) surface [18,22].

Based on the previous work of our group, this paper aims at simulating the wetting processes of Li droplet on Fe (1 0 0), (1 1 0), (1 1 2) and polycrystalline Fe surfaces and discussing the wetting characteristics of the Li-Fe solid–liquid systems in detail. The time-dependent contact angle  $\theta(t)$  and precursor film radius  $R(t)$  were measured to express the wettability of Li droplet on Fe (1 0 0), (1 1 0) and (1 1 2) surfaces. A new method (the time-dependent contact atom number) was proposed to describe the wetting of Li droplet on Fe substrates from microscopic level, and the wetting behavior difference between the single crystal and polycrystalline Fe surfaces was discussed. The effect of temperature on the wetting property was also researched.

## 2. Simulation model and method

The interatomic interactions for Li-Li, Fe-Fe and Li-Fe are represented by the modified analytic embedded-atom method (MAEAM) potential, which has been constructed by our group, and the potential formula and parameters can be found in previous papers [32–34]. Based on these potentials, the properties of Fe (0 0 1)-Li solid-liquid interface and the clustering processes of Fe atoms in liquid Li at different temperatures have been well described [34,35]. In this paper, all the molecular dynamics simulations were performed using the parallel code LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) [36], with a timestep of 1 fs. The Parrinello-Rahman barostat [37] and the Nose-Hoover thermostat [38,39] were implemented to control the pressure and temperature, respectively.

In our simulations, the initial configurations of a Li droplet placed on a surface of Fe substrate were generated as follows. Three BCC Fe crystals with the (1 0 0), (1 1 0) and (1 1 2) surface normal to the z axis were constructed as the substrates, respectively. Take the Fe (1 0 0) substrate as an example, the simulation box was constructed with a size

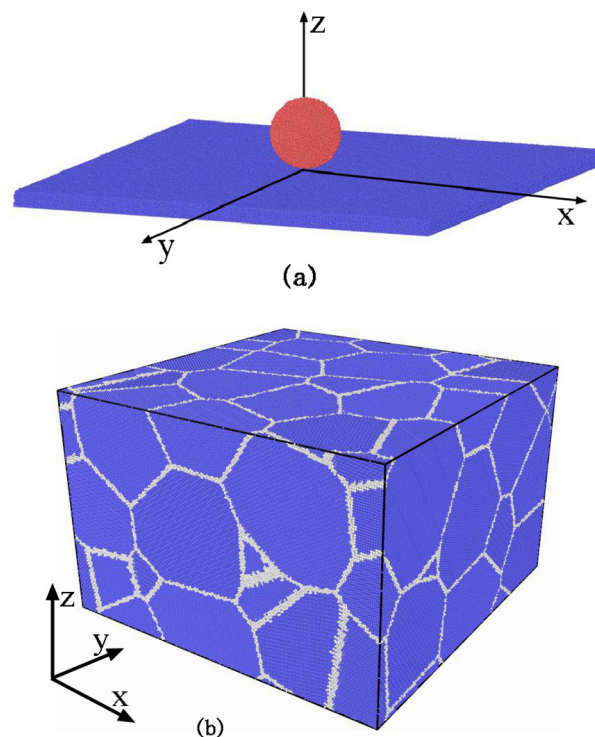


Fig. 1. (a) Schematic illustration of initial configuration of the wetting systems. The red sphere represents a Li droplet, and the blue slab represents the Fe substrate. (b) Initial structure of the 3-D polycrystalline Fe. The blue atoms are the grain atoms, while the white atoms denote the grain boundaries atoms.

of  $160a \times 160a \times 6a$  ( $a$  is the lattice constant, determined by a separate simulation in NPT ensemble at corresponding temperature) in the x, y, and z directions. Periodic boundary conditions (PBC) were applied in the x and y directions (parallel to the surface), and an open boundary conditions were used along the z direction. The substrate thickness in z was 12 Fe (1 0 0) atomic layers, and the substrate contained 400,722 Fe atoms. The model of Fe (1 1 0) and Fe (1 1 2) substrates were also constructed using the same method. Then, a Li droplet was put on the substrates, made up an initial simulation system. To prepare the Li droplets, one cubic Li bcc crystal with side length of 142.16 Å was melted and equilibrated in NPT ensembles at 460 K, 500 K and 800 K, respectively. Then, the spherical liquid droplet with radius about 40 Å consisting of 11,922 Li atoms was cut out and placed on the top of the prepared substrates. The bottom of the Li droplet was positioned about 2.5 Å above the substrate surface. The initial configuration of the system were built with the above parameters, are present in Fig. 1(a). All subsequent simulations of wetting process were performed in NVT ensembles at a corresponding temperature. In the simulation of wetting process, the lowest two layer Fe atoms in the substrate were fixed rigidly throughout the entire simulations process, whereas the other atoms were permitted to relax. The following calculations of the wetting were studied after the relaxed configurations. The time-dependent radius  $R(t)$  and dynamic contact angle  $\theta(t)$  of the spreading Li droplet were calculated to describe the wetting characteristics. In addition, to investigate the wetting behavior of Li on polycrystalline Fe surface, a polycrystalline Fe sample with a size of  $460 \text{ \AA} \times 460 \text{ \AA} \times 300 \text{ \AA}$  was generated by Voronoi cell method, and it consisted of 27 grains, as shown in Fig. 1(b). The relatively stable sample was first obtained through an energy minimization procedure, and then equilibrated 0.8 ns using NPT ensemble at the corresponding temperature. In order to reduce the computation cost, the substrate samples used to study the wetting process of Li droplet on polycrystalline Fe surfaces were generated by cutting a slab of the thickness of 42 Å (along the z direction). The polycrystalline Fe slab included 736,326 atoms and was relaxed to

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