



Molecular dynamics study of stable and undercooled liquid zirconium based on MEAM interatomic potential

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ABSTRACT

Large scale molecular dynamics simulations with two different embedded atom method (MEAM) potentials are applied to investigate the structural and dynamic properties of stable and undercooled liquid zirconium. Simulation shows that MEAM model of zirconium constructed on the basis of a bcc structure is more successful than the MEAM model in the framework of an hcp structure in predicting the structural properties of liquid zirconium. We report calculated values of the melting point, self-diffusion coefficient, mean square displacement, pair correlation function and bond angle distribution function. The short range order (SRO) in the stable and undercooled liquid is also examined. We analyze the three-dimensional SRO by the means of a Common Neighbours Analysis. The simulated properties of liquid zirconium are compared with experimental data available and first principle molecular dynamics results. Comparisons show reasonable agreement between the simulated results from MEAM model based on the basis of a bcc structure and experimental data.

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1. Introduction

Computer simulations such as molecular dynamics simulation provide a physical insight into understanding various phenomena on the atomic scale and enable one to predict some thermodynamic, mechanical, structural, transport and dynamic properties of materials. MD simulations nowadays come in two main varieties. Classical molecular dynamics (MD) simulations involve classical interaction potentials between the particles in the simulation box. These potentials are either derived from first principle calculations or fitted to certain experimental data. Ab initio molecular dynamics (AIMD) simulations, on the other hand, are based on first principles: at every time step in the simulation, the electronic structure is calculated, typically by using the density functional theory (DFT) formalism. First principle calculations can provide the most reliable interatomic potential. However, realistic simulations of some properties often require the presence of a number of atoms which renders these methods impractical. One alternative is to use semi-empirical potentials. A recent paper on liquid nickel [1] has demonstrated that semi-empirical potentials can lead to a close agreement with first principles calculation. Thus, MD and AIMD could provide the same results.

Zirconium and zirconium alloys have a wide range of technological application as high temperature materials, nuclear and

amorphous materials. There is a great deal of interest in predicting the local structure and dynamic properties of stable and undercooled liquid Zr. The present work aims to carry out a MD study of the structural and dynamic properties of liquid and undercooled zirconium. In this study, among all the semi-empirical potential available in the literature, we use the MEAM model proposed initially by Baskes et al. [2,3] because it is one of the most accepted methods to study physical properties of liquid metal. For some liquid metals, this method has been used by Baskes and co-workers [4–6] to calculate the static structure factor, the pair correlation function, melting points and transport coefficients (self-diffusivity and viscosity).

When heated to temperatures higher than about 1135 K zirconium transforms from an hcp to a bcc structure. This is a first order martensitic transition, which proceeds via the Nishayama–Wassermann mechanism. A first order liquid transition occurs at about 2125 K. Jakse et al. carried out the AIMD study of the structural properties of stable and undercooled liquid zirconium [7–9] and they pointed out that around the melting point the local structure of liquid and undercooled zirconium is closer to a bcc-like structure than a hcp-like structure. Thus, in the calculation of structural properties of liquid zirconium it is probably preferable to use interatomic potential with bcc as reference structure. Unfortunately, currently in the literature only the MEAM potential of zirconium with hcp as reference structure is available [3,10,11].

In this paper we constructed a new zirconium potential on the basis of a bcc structure. The calculation of the parameters of the potential is done according to the Baskes scheme [2,12]. The validity of the new potential is examined by calculating several properties

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of bcc-Zr such as elastic constants, vacancy formation energy, structural energy difference and the results are compared with ab initio calculation and the available experimental data. Subsequently, the potential is used to carry out a MD study of the structural and dynamic properties of liquid and undercooled zirconium. We compare our simulation results with AIMD simulation data [7–9] and develop an analysis that is as free of subjective parameters as possible. MD simulations are also useful for understanding the nucleation and crystallization of materials. The dynamics of the nucleation process and the structure generated during crystallization of zirconium are not discussed in this study. However, we will show that the MEAM potential with bcc as reference structure, developed in this work, is also useful for investigating the crystallization of zirconium.

This paper is layed out as follow: Section 2 is devoted to describing the interaction model for bcc zirconium and relevant equations are shown. In Section 3 we give a brief but important description of computational details. In Section 4, the results obtained are shown and compared with available experiment data and previous ab initio calculation [7–9]. Finally, in Section 5 we give the conclusions of this work.

2. Modified embedded atom method potential for bcc zirconium

The total energy E of a system of monatomic atoms in the MEAM formalism [2,3,10] can be written as follows

$$E = \sum_i E_i \quad (1)$$

with

$$E_i = F_i(\bar{\rho}_i) + \frac{1}{2} \Phi_i \quad (2)$$

Here, E_i denotes the energy of atom i , F is the embedded function, which depends on the background electron density $\bar{\rho}_i$ at site i and Φ_i denotes the mean of the total pair potential which is given by

$$\Phi_i = \sum_{i \neq j} \phi_{ij}(R_{ij}) \quad (3)$$

where Φ_{ij} is the pair interaction between atoms i and j and R_{ij} is the distance between atoms i and j . The embedded function F is the energy required to embed an atom into the electron sea (background electron density) constituted by all other atoms of the system. According to Baskes et al. F is formulated as

$$F(\bar{\rho}_i) = A_i E_i^0 \bar{\rho}_i \ln \bar{\rho}_i \quad (4)$$

Here, A_i is an adjustable parameter and E_i^0 is the sublimation energy of the reference structure. The background electron density can be obtained from the partial electron densities as

$$\bar{\rho}_i = \frac{\bar{\rho}_i^0}{\rho_i^0} (1 + \Gamma_i) \quad (5)$$

with

$$\Gamma_i = \sum_{l=1}^3 t^{(l)} \left(\frac{\rho_i^{(l)}}{\rho_i^{(0)}} \right)^2 \quad (6)$$

The background electron density $\bar{\rho}_i$ is assumed to be a function of partial electron densities $\rho_i^{(l)}$, $l=0-3$ which is written as

$$\bar{\rho}_i^{(0)} = \sum_{j \neq i} \rho_j^{a(0)}(R_{ij}) S_{ij} \quad (7.a)$$

$$(\bar{\rho}_i^{(1)})^2 = \sum_{\alpha=1}^3 \left[\sum_{j \neq i} x_{ij}^\alpha \rho_j^{a(1)}(R_{ij}) S_{ij} \right]^2 \quad (7.b)$$

$$(\bar{\rho}_i^{(2)})^2 = \sum_{\alpha, \beta=1}^3 \left[\sum_{j \neq i} x_{ij}^\alpha x_{ij}^\beta \rho_j^{a(2)}(R_{ij}) S_{ij} \right]^2 - \frac{1}{3} \left[\sum_{j \neq i} \rho_j^{a(2)}(R_{ij}) S_{ij} \right]^2 \quad (7.c)$$

$$(\bar{\rho}_i^{(3)})^2 = \sum_{\alpha, \beta, \gamma=1}^3 \left[\sum_{j \neq i} x_{ij}^\alpha x_{ij}^\beta x_{ij}^\gamma \rho_j^{a(3)}(R_{ij}) S_{ij} \right]^2 \quad (7.d)$$

with

$$x_{ij}^\alpha = \frac{R_{ij}^\alpha}{R_{ij}} \quad (7.e)$$

where α , β and γ denote the components of the distance vector between the atoms j and i . R_{ij}^α is the α -component of the distance vector between atoms j and i . The $\rho_i^{a(l)}(R_{ij})$, $l=0-3$ are the partial atomic electron densities that are contributed by the atom j at the distance R_{ij} from site i . The equations of the partial atomic electron density have been assumed to be given by a simple exponential form

$$\rho_i^{a(l)}(R_{ij}) = \rho_i^0 \exp \left[-\beta_i^{(l)} \left(\frac{R_{ij}}{R_i^0} - 1 \right) \right] \quad (8)$$

where R^0 denotes the equilibrium nearest neighbour distance in the bulk of a perfect crystal, and $\beta_i^{(l)}$ $l=0-3$ the exponential decay factor for the atomic densities. The screening function $S_{ij} = \prod_{k \neq i, j} S_{ijk}$ is introduced to account for relative contributions from atoms at different locations and can be considered as a forced cut-off technique. It is given by

$$S_{ijk} = \begin{cases} 0 & \text{for } C_{ijk} \leq C_{\min,ijk} \\ \left[1 - \left(\frac{C_{\max,ijk} - C_{ijk}}{C_{\max,ijk} - C_{\min,ijk}} \right)^4 \right]^2 & \text{for } C_{\min,ijk} \leq C \leq C_{\max,ijk} \\ 1 & \text{for } C_{ijk} \geq C_{\max} \end{cases} \quad (9)$$

where

$$C_{ijk} = 1 + 2 \frac{r_{jk}^2 r_{ji}^2 + r_{ki}^2 r_{ji}^2 - r_{ji}^4}{r_{ji}^4 - (r_{jk}^2 - r_{ki}^2)^2} \quad (10)$$

In order to determine the pair interaction ϕ_{ij} , we consider the reference structure as a homogenous monatomic solid with interaction limited to the first neighbours only. In the reference structure, ϕ_{ij} can be quite easily obtained by using Eqs. (2) and (3)

$$\phi_{ij} = \frac{2}{Z_i} \left[E_i^u(R_{ij}) - F_i \left(\frac{\bar{\rho}_i^0}{Z_i} \right) \right] \quad (11)$$

where $\bar{\rho}_i^0$ is the background electron density for the reference structure, Z_i is the number of nearest neighbours in the bulk of a perfect lattice and E_i^u is the energy per atom for the reference structure as a function of the nearest neighbour distance R_{ij} given by the universal energy function proposed by Rose et al. [13].

$$E_i^u(R_{ij}) = -E_i^0 \left[1 + \alpha_i \left(\frac{R_{ij}}{R_i^0} - 1 \right) \right] \exp \left[-\alpha_i \left(\frac{R_{ij}}{R_i^0} - 1 \right) \right] \quad (12)$$

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