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Molecular dynamical simulation of the structural and melting properties of Al_{196} cluster

Chun-Li Li, Mailitan Kailaimu, and Hai-Ming Duan*

College of Physical Science and Technology, Xinjiang University, Urumqi 830046, China

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Abstract. Based on the Gupta-type semi-empirical inter-atomic many-body potential, the melting behaviors of the Al_{196} cluster are systematically studied by using the molecular dynamics method combined with the annealing and quenching techniques. Our simulation results show that from different initial structures one can observe quite different melting behaviors. From a relatively low-energy stable geometry, two peaks occur clearly in the heat capacity curve; But only one peak dominates the heat capacity curve if starting from the ground-state or its closer low energy structures. Reasons of the different melting properties of the Al_{196} cluster are explored by analyzing the energy distributions of the simulated quenching structures of Al_{196} at different temperatures.

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Key words: Gupta potential, cluster, molecular dynamics, melting

1 Introduction

Clusters are aggregates composed of several to thousands of atoms (molecules) bonding in certain physical or chemical forces, that exist stably in microscopic state [1]. It has been aroused a great interest, just because of its unique physical and chemical properties and potential applications in many fields such as the new material physics, the nano-electronics and the nano-catalyst [2-14]. It has already become a new and significantly important field to study the formation, structures, properties and evolution behaviors of clusters. The melting behaviors of clusters are completely different from that of the bulk materials, and the melting points of clusters usually decrease with decreasing the cluster size, and moreover, there are apparent premelting temperature intervals of clusters. For the small clusters their melting behaviors are accompanied by obvious size effects.

*Corresponding author. *Email address:* dhm@xju.edu.cn (H. M. Duan)

For example, the experimental study of the melting behaviors of simple monovalent Na clusters [11] show that the melting points of clusters change nonmonotonously (oscillatorily) of the clusters containing less than 200 atoms, and the negative heat capacity has been observed for Na_{147} cluster [12]. Some exotic behaviors are also observed, for example, for the simple trivalent Ga clusters in a small size regime, the melting temperatures are observed to be higher than the bulk melting point [13-14]. The preeminent heat conductivity and malleability of trivalent aluminum crystal have brought extensive applications in social practice, and the study of aluminum clusters has also revealed a series of singular behaviors. For example, the ferromagnetic properties of extremely small aluminum cluster [15], and the super-stability of Al_{13}^{-} cluster which can provide a great potential as being cluster-assembled materials [16], and the good performance in catalyst [17]. Recently, Jarrold and co-workers have conducted plenty of experiments on the melting properties of small and medium-sized Al_n ($n<200$) cluster and observed generally irregular phenomenon on the heat capacity curves of small-sized Al_n ($n<100$) clusters [18] (if the heat capacity curve has no clear peak, then considered irregular). Moreover, a double-peak feature in heat capacity has been clearly observed for some larger-sized Al_n ($n>100$) clusters, and the authors also conjectured the reason of the double-peak [19], but still lack of specific dynamic description at atomic level (like molecular dynamics simulation study).

In this paper, by using the molecular dynamics method based on the semi-empirical Gupta interatomic potential combined with the molecular dynamics simulated annealing and quenching techniques, the melting behaviors of Al_n cluster are systematically studied, and the origin and reason of different melting behaviors of Al_n cluster are also analyzed in detail by the potential energy distributions at different temperatures.

2 Computational methods

2.1 Potential function

The interaction between atoms, which is depicted by the potential function, is the fundamental to determine the dynamic behaviors of clusters. In this letter, the interaction between atoms of Al clusters are described by using the semi-empirical many body Gupta potential based on the embedded-atom potential and tight-binding model of the second moment approximation, in which the potential parameters are obtained from fitting the relevant physical parameters of crystal (cohesive energy, lattice constant and elastic moduli, etc). Moreover, this kind of many body potential has been extensively used to study the geometries [20-21] and dynamic behaviors [22] of the metal and alloy clusters. Gupta potential can be written as the sum of a Born-Mayer type repulsive part and a many-body attractive part, as shown below:

$$V=\sum_i\Big(\sum_{j(\neq i)} A\exp[-p(\frac{r_{ij}}{r_0}-1)]-\sqrt{\sum_{j(\neq i)} B^2\exp[-2q(\frac{r_{ij}}{r_0}-1)]}\Big) \tag{1}$$