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Molecular Dynamics Study of Al_{147} Melting

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Abstract: The melting behavior of a particle in nanometer size attracts many attentions in material science. Many experimental studies of melting transition of sodium cluster, gallium, sodium chloride, and aluminium (Al) cluster have been reported. Al_{147} cluster is one of the special Al cluster that form icosahedral structures at ground state. We study the structural change of this cluster on various temperatures using molecular dynamics simulation. The melting behavior is investigated using Lindemann index, which represent the amplitude motion of the atoms from its original position. We obtained from the calculation that the melting temperature of Al_{147} cluster is approximately 700 K.

Keywords: *Melting, Al_{147} Cluster, Molecular Dynamics Simulation, Lindemann Index*

Introduction:

Cluster material has attracted a lot of attention from the researchers due to its potential applications in electronic devices and chemical sensors [1]. Since cluster has higher surface:volume ratio than bulk materials, it is widely used as catalyst. It has been known that some materials such as carbon nanotubes (CNTs) and carbon fibers have been successfully grown via catalytic chemical vapour deposition (CCVD) technique [2,3]. The metal cluster has been used as the catalyst for the reaction. Several studies have been performed to investigate mechanism of the dissociation reaction of carbon precursor molecules (such as hydrocarbon) on the metal cluster or surface at high temperatures [4,5]. The high temperature normally enhances the reaction rate. Therefore, it is important to investigate the behaviour of the cluster at various temperatures. Al_{147} is one of the special cluster which exist in regular icosahedral structure. This study is aimed to elucidate the melting behaviour of Al_{147} cluster using molecular dynamics simulation.

Computational Methods:

The simulation system consists of 147 Al atoms forming icosahedral structure as shown in Fig. 1. The dimension of simulation box is $40.0 \times 40.0 \times 40.0$ Å^3 in *x*-, *y*-, and *z*- dimensions, respectively. The embedded atom method (EAM) of Zope and Mishin [6] is employed to describe the interactions between Al atoms. This potential has been used in our previous study. It has been proven that the melting temperature of Al bulk from our calculation is in reasonable agreement with the experimental value [7].

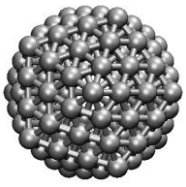

Figure 1: Initial configuration of Al_{147} cluster

The series of MD simulations are performed at the temperature range from 300 K until 1500 K increased every 100 K. The systemic equilibration and the statistical average have been done for 990 ps and 10 ps, respectively. The NVT Nosé-Hoover method [8] has been used to control the temperature. In order to investigate the amplitude motion of the atoms, the local Lindemann indices δ_i are calculated at each temperature as [9]:

$$\delta_i = \frac{1}{N-1} \sum_{j(\neq i)} \frac{\sqrt{\langle r_{ij}^2 \rangle_T - \langle r_{ij} \rangle_T^2}}{\langle r_{ij} \rangle_T}$$

$$\delta = \frac{1}{N} \sum_i \delta_i$$

where δ_i and δ are the Lindemann indices of *i*th atoms and cluster, respectively. The angle bracket $\langle \cdots \rangle_T$ denotes the time average at the temperature T.r_{ij} is the distance between *i*th and *j*th atoms and N is the number of atoms in the cluster.

Results and Discussion:

In this section, the melting behaviour of Al_{147} cluster analysed using Lindemann index is presented and discussed thoroughly.

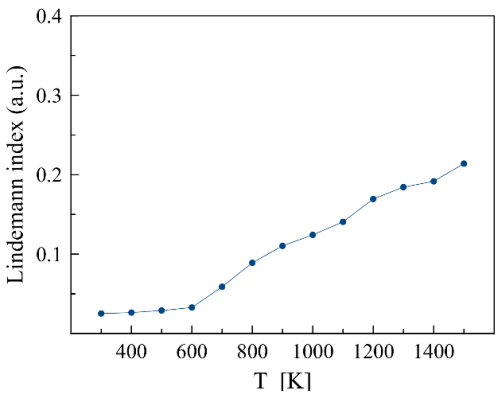

Figure 2: Temperature dependence of average Lindemann index of Al_{147} cluster

Figure 2 shows the temperature dependence of average Lindemann index of Al_{147} cluster. At the temperature 300 K to 600 K, the value of Lindemann indices are increasing slowly. There is a sudden jump in value of Lindemaan index at temperature 700 K. It also can be seen from the figure that Lindemann index increase rapidly at higher temperature. This indicates that the atoms become more active at higher temperature.

The behaviour of the atoms during the melting process is shown in Fig. 3. At the temperature 300 K until 600 K, the atoms maintain its original position relative to the center of mass. Suddenly, the position of atoms spread irregularly at 700 K and 1500 K as well.

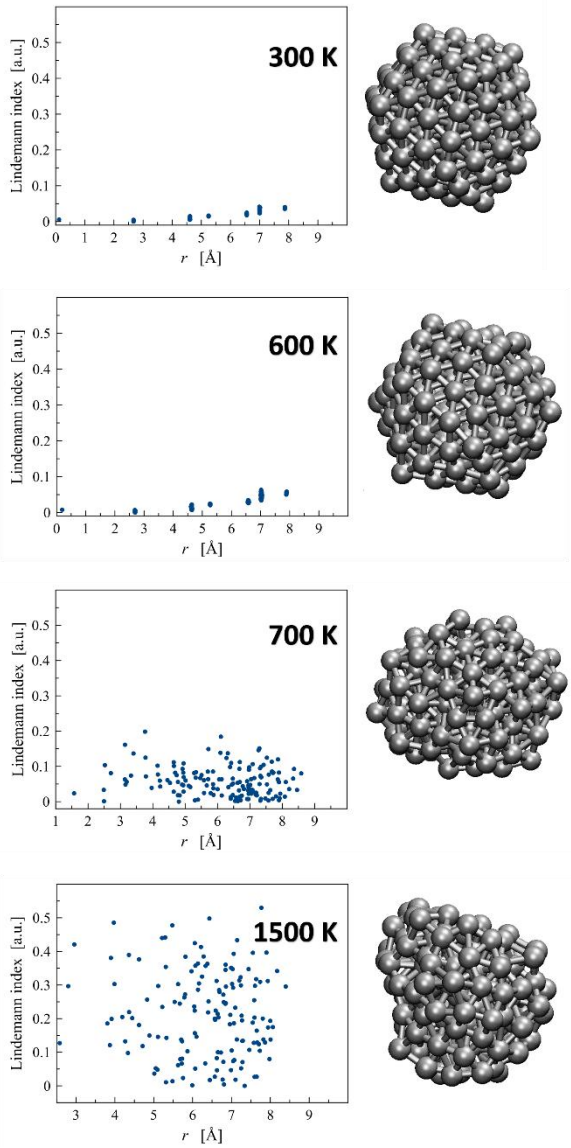

Figure 3: Radial distribution of the Lindemann indices of the atoms in Al_{147} cluster at different temperatures (left) and snapshot of the cluster at different temperatures (right). r is the average radius of the atoms from center of mass.

From Fig. 3 it can be seen that the Lindemann indices of the atoms are also increasing rapidly at 700 K. The high Lindemann indices are not only found in the surface atoms, but also in the inner atoms of the cluster. In the right panel of Fig. 3, we can seethat shape of icosahedral cluster are maintained at 300 K and 600 K. At 700 K and 1500 K, the shapes change to the irregular structure. These facts show the evidence that the melting of Al_{147} cluster occurs at 700 K.

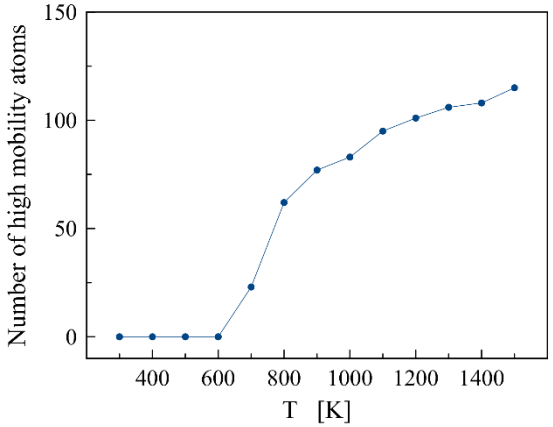

Figure 3: Temperature dependence of number of atoms having large amplitude motion ($\delta \geq 0.1$)

Figure 3 shows the temperature dependence of number of high mobility atom ($\delta \geq 0.1$). At the temperature 600 K or less, all the atoms in the cluster have the Lindemann indices less than 0.1. The population of high mobility atoms increase to around 17 % of the total atoms at 700 K. At the higher temperature, the number high mobility atoms are growing.

Conclusion:

The MD simulation has been carried out to investigate the melting behaviour of Al_{147} cluster. The Lindemann index is used to analyse the diffusion of the atoms. It is found that the melting temperature Al_{147} cluster is around 700 K.

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