

Cluster on the fcc(111) surface: structure, stability and diffusion

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Abstract

The static and dynamical properties of a highly symmetric cluster on a fcc(111) surface are studied using the molecular-dynamics method. We find that the cluster can only be stable on the surface up to a certain temperature much lower than the melting temperature of the corresponding isolated cluster; the surface can strongly change the thermal properties of the cluster. The fast diffusion of the cluster is attributed to the rolling of cluster as a whole on the surface, and the dependence of diffusion constants on the structural mismatch is also studied. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: Cluster; Diffusion and migration; Molecular dynamics

1. Introduction

In the past decade, cluster science is one of the important fields for physicists, chemists and material scientists. Much research effort has been devoted to the studies of the physical and chemical properties of isolated clusters. It has been found that clusters can display a variety of so-called finite size effects. Recently, intensive research effort is moved to the design and fabrication of the materials which are assembled from clusters [1–9], because such materials could exhibit many interesting and useful physical properties. For example, the close-packed planar arrays of gold clusters can display the Coulomb charging behavior [1]. The experimental work for the cluster supported on surface stimulates further theoretical study and computer simulation.

There have been several computer simulations about the structure and stability of clusters supported on surface. Blaisten-Barojas et al. studied the thermal behavior of a Lennard–Jones (LJ) cluster on a continuous surface [10]. The structure and stability of $(C_{60})_n$ clusters on surface have also been investigated by using the modified LJ potential [11–14]. However, in those studies where the atomic structure of the surface was treated as a rigid and structureless continuous plane, we have shown that this simplification could be questionable [15]. Using the molecular-dynamics (MD) simulation, several authors studied the structure and stability of a cluster as it approaching to a surface for specific materials [16–21]. Based on first-principle calculations, Hakkinen and Manninen found that the stability of the magic Na_8 cluster is strongly dependent on the surface [22]. All these studies showed that the surface can play an important role in the structure and stability of clusters.

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The other important issue concerning cluster-surface system is clusters diffusion on surfaces [23–42]. Most of the recent theoretical studies [26–34] have focused on the two-dimensional cluster epitaxially oriented on the surface, and found very low diffusion coefficients with order $10^{-17} \text{ cm}^2 \text{ s}^{-1}$. This kind of diffusion is related to the single-atom [26–32] or dislocation mechanisms [33,34]. In contrast, recently Bardotti et al. [35,36] have shown experimentally that large (a hundred to a few thousand atoms) three-dimensional clusters, even a microcrystal, can have a high diffusion coefficient at room temperature. This work is reminiscent of early work [37–41]. Theoretical [42] and experimental [37–41] work suggested that the fast diffusion of the larger three-dimensional cluster may be attributed to the translation motion of the cluster as a whole. It is also found that, during the motion, cluster may rotate as entities on the surface. The translation and rotation as entities are basically different from the so-called dislocation mechanism for two-dimensional clusters. For the dislocation mechanism, the cluster diffuses by the motion of the dislocation involved in the cluster; however, for translation and rotation as entities, no dislocation in the cluster contributes to the diffusion.

In this paper, by explicitly considering the atomic structure of the cluster and the surface, we study the structure, stability and diffusion for a highly symmetric cluster on the fcc(111) surface. We believe that our studies can shed light on understanding of the diffusion process for the cluster on the surface.

In the rest of this paper, we present the calculation details in Section 2, and Section 3 includes the main results and discussion, finally, we summarize the major conclusion in Section 4.

2. Calculation details

In this paper, we study the structure and thermal behavior for an icosahedral (I_h) 13-atom cluster on fcc(111) surface, with particular emphasis on the general properties for the cluster being stable on the surface. The calculations are performed on the surface consisting of five layers of atoms, in

which each layer contains 100 atoms. The atoms in the bottom two layers are kept fixed to mimic the semi-infinite solid, all the rest are allowed to move. The periodic boundary conditions are imposed in the directions parallel to the surface. Temperature is controlled by scaling the velocity of atoms in the third layer. To see the influence of the system size on the results, we have repeated a few calculations on a larger surface, which consists of six layers of atoms and each layer contains 256 atoms. The calculations show that the system size does not change the results significantly.

The atoms in the cluster and surface interact through LJ type potentials. Empirical potential of this type, originally developed for describing the inert gases, is now commonly used to model the general properties of condensed systems [42]. In the present simulation, the interatomic LJ potential ϕ reads:

$$\phi_{\alpha\beta}(r) = 4\epsilon_{\alpha\beta} \left[\left(\frac{\sigma_{\alpha\beta}}{r} \right)^{12} - \left(\frac{\sigma_{\alpha\beta}}{r} \right)^6 \right], \quad (1)$$

where α and β denote the atom A in the cluster and the atom B on the surface, respectively. Reduced units are used in this paper, that is, σ for length, ϵ for energy, $\tau = (m\sigma^2/\epsilon)^{1/2}$ for time, and $T = K_B T/\epsilon$ for the temperature, where K_B is the Boltzmann constant and m is the mass of atoms. The reduced unit for the diffusion constants is σ^2/τ . In all of calculations, we assume $\sigma_{BB} = 1.0$, $\sigma_{AB} = \frac{1}{2}(\sigma_{AA} + \sigma_{BB})$ and $\epsilon_{AA} = \epsilon_{BB} = 1.0$. The potential cuts off at $r_c = 2.5 \sigma_{\alpha\beta}$. Our simulation uses the standard constant-energy MD technique. The equations of motion are integrated using the Verlet method [43].

To quantitatively characterize structural changes, we calculate the deformation energy of the cluster, E_d , which is defined by

$$E_d = E_{13}^d - E_{13}^0, \quad (2)$$

where E_{13}^0 is the total energy of the isolated I_h cluster, E_{13}^d is the total energy of the cluster when it is on the surface. The interaction energy between the cluster and the surface, E_i , is also defined by

$$E_i = \sum_{i=1}^{N_A} \sum_{j=1}^{N_B} \phi_{AB}(r_{ij}). \quad (3)$$

The motion of the cluster as a whole has been investigated by calculating the diffusion constant D , which is obtained from the mean-square-displacement of the mass center

$$\langle \mathbf{R}^2(t) \rangle = \langle [\mathbf{R}(t + t_0) - \mathbf{R}(t_0)]^2 \rangle_{t_0}. \quad (4)$$

Using the Einstein relation, we can obtain the diffusion constant for the cluster

$$D = \lim_{t \rightarrow +\infty} \frac{\langle \mathbf{R}^2(t) \rangle}{4t}, \quad (5)$$

where $\mathbf{R}(t)$ is the coordinate of the mass center of the cluster.

Typically, the length of the simulation time used to calculate thermal properties and diffusion constant are ca. 5×10^4 and 2×10^5 MD steps, respectively.

3. Results and discussion

3.1. Structural properties

In contrast to an atom on the surface in which the structure is essentially determined by the position of the adatom, a cluster on the surface may have a complicated structure, since the orientation of the cluster to the surface may play an important role as the cluster approaching to the surface. The importance of structure orientation has been observed in the previous study on clusters [15,44–46]. To determine the structure of the cluster on surface, we have chosen several initial configurations with different orientations to the surface. By performing the steepest-descent, two different structures, with the cluster slightly deformed, are obtained for $\epsilon_{AB}=1.0$ and $\sigma_{AA}=1.0$. In the first obtained structure (labeled as A), one of the 20 triangle faces of the cluster is parallel to the surface, and the three bottom atoms of the cluster are at hcp sites of the surface. In another structure (labeled as B), there are also three atoms at the interface, which occupy three fcc sites of the surface. But the bottom face of the cluster is tilted to the surface, instead of parallel to the surface. The structure B is similar to what obtained for the same cluster on fcc(100) surface [15].

We take structure A as an example to study the influence of different ϵ_{AB} and σ_{AA} on the cluster. For each $\epsilon_{AB}=0.5, 0.65, 0.8, 1.0$ and 1.2 , σ_{AA} is changed from 0.6 to 1.4 . We find that the cluster can be supported on the surface for all the studied ϵ_{AB} and σ_{AA} although the deformation can be existed. In Fig. 1, we show the deformation energy E_d as a function of σ_{AA} for several ϵ_{AB} . It is easy to understand that, the smaller ϵ_{AB} is, the smaller E_d is. As $\epsilon_{AB}=0.5$, the deformation energy is only ca. 0.2% of the total energy of cluster, but for $\epsilon_{AB}=1.2$, E_d reaches 4% of the total energy of the cluster. The behavior of the deformation energy changing with σ_{AA} is similar for different ϵ_{AB} . For all ϵ_{AB} , E_d has a minimum ca. $\sigma_{AA}=1.0$, and a maximum at $\sigma_{AA}=0.7$ can clearly be observed. For σ_{AA} ca. 1.0 , the structure of cluster can well match fcc(111) surface. The bottom triangle face of the cluster can be at the ideal fcc position. So the stress in the interface is very small, which leads to small deformation on the cluster. Whatever σ_{AA} is departing from 1.0 , the stress in the interface will increase, which will result in a larger deformation. When σ_{AA} decreases to ca. 0.7 , the bottom triangle face of undistorted cluster has difficulty in finding a suitable position. The three bottom atoms of the cluster cannot sit at either the hcp or fcc sites simultaneously. It is not favorable on energy consumption, so the large deformation is expected for

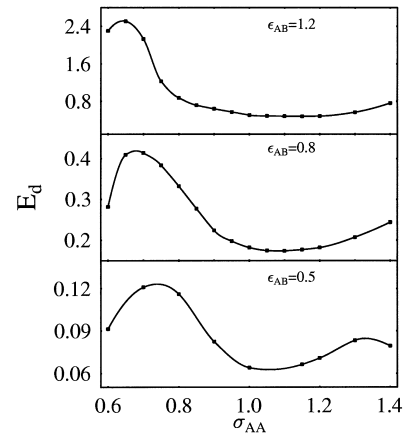


Fig. 1. The deformation energy E_d of the cluster in structure A as a function of σ_{AA} for several ϵ_{AB} . For different ϵ_{AB} , the change of E_d in responding to the change of σ_{AA} is similar, all of them reach a maximum at σ_{AA} ca. 0.7 .

$\sigma_{AA}=0.7$. With $\sigma_{AA}<0.7$, the cluster could match the surface with one bottom atom at the hcp site and other two at the fcc site, so the deformation decreases again. The deformation of the cluster is evidently different on both sides of the commensurate ($\sigma_{AA}=1.0$). As $\sigma_{AA}\leq 1.0$, E_d is larger than that for $\sigma_{AA}>1.0$. For smaller ϵ_{AB} , E_d will reach another maximum at σ_{AA} ca. 1.3. These results indicate that the shape of E_d changing with σ_{AA} is weakly dependent on ϵ_{AB} .

In Fig. 2, we present the interaction energy E_I as a function of σ_{AA} . For comparison, E_I has been renormalized by ϵ_{AB} . For small ϵ_{AB} (~ 0.5), E_I almost decreases linearly with the increasing of σ_{AA} . For large ϵ_{AB} ($\sim 0.8, 1.2$), the shape of E_I is similar to that for smaller ϵ_{AB} (~ 0.5) as $\sigma_{AA}>0.8$, but E_I has significantly decreases ca. $\sigma_{AA}=0.7$ with respect to the linear-like behavior of small ϵ_{AB} (~ 0.5). The different behavior of E_I for different ϵ_{AB} could be attributed to large deformation at σ_{AA} ca. 0.7 for large ϵ_{AB} , which results in a sudden decrease of E_I .

3.2. Thermal stability

To investigate the thermal stability of the cluster on the surface, we choose $\epsilon_{AB}=0.5, 0.8$ and 1.0 , and for each ϵ_{AB} , σ_{AA} is changed from 0.5 to 1.2 . Fig. 3 shows the interaction energy E_I (right scale) and the distance d between the mass center of the cluster to the surface (left scale) as a function of

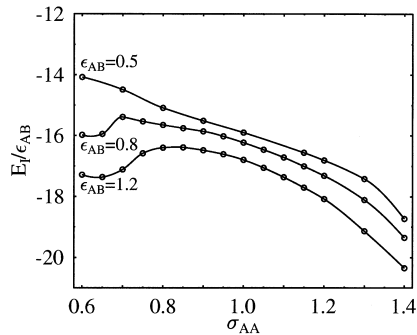


Fig. 2. The interaction energy E_I as a function of σ_{AA} for the cluster in structure A at zero temperature. For small ϵ_{AB} , E_I almost decreases linearly with the increasing of σ_{AA} , but for large ϵ_{AB} , the change of E_I versus σ_{AA} has evident deviation from the linear behavior.

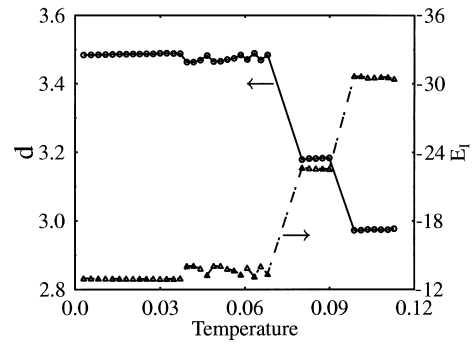


Fig. 3. The distance d of the cluster center to the surface and the interaction energy E_I as a function of temperature with $\epsilon_{AB}=0.8$, $\sigma_{AA}=1.0$. At $T=0.07$, the sudden changes of E_I and d indicate that the cluster has collapsed.

the temperature. We find that, at the temperature $T_c=0.07$, E_I and d suddenly change. The significant decreasing of E_I indicates that the interface between the cluster and surface becomes large, and the sudden decrease of d indicates the collapse of the cluster. These results imply that the structure of cluster has been changed above T_c . Visual observation demonstrates that, at the temperature lower than T_c , the cluster almost maintains its structural character, at the temperature above T_c , the cluster begins to collapse. Upon heating, the cluster collapses step by step. Fig. 4 shows some snapshots of the cluster on surface during this heating process. Up to $T=0.07$ (Fig. 4a), the cluster exhibits no more than slight deformation with respect to the structure of the cluster on the surface at $T=0$, but at $T=0.08$, it has collapsed (Fig. 4b) on the surface. Upon heating to $T=0.11$, the cluster collapses further (Fig. 4c). It is necessary to point out that, if we heat the system further, we have not found the liquid-like phase in the cluster before it totally spreads out on the surface. Similar behavior has been observed for all the studied ϵ_{AB} and σ_{AA} .

We note that the present results are different from the previous results, in which the cluster was found to be stable on the surface up to very high temperature, even higher than the melting temperature of the free 13-atom LJ cluster [10]. Since the energy transfer and the vibrational coupling between the surface and the cluster are important, as pointed out previously [15,42], we can attribute

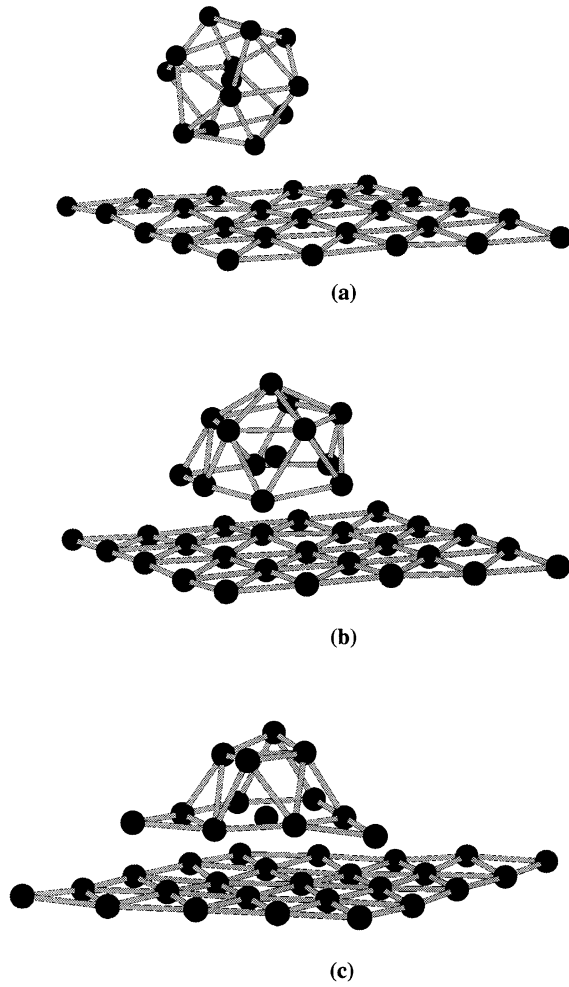


Fig. 4. The snapshots of the cluster on the surface at $T=0.06$ (a), 0.08 (b) and 0.11 (c) for $\epsilon_{AB}=0.8$, $\sigma_{AA}=1.0$. As temperature lower than T_c (0.07), the cluster maintains its individual characters, and collapses on the surface for temperature higher than T_c .

the difference between our results and previous results [10] to the structureless surface used by Blaisten-Barojas et al. [10].

The interaction between surface and cluster is very important for the stability of cluster on the surface. Fig. 5 shows T_c as a function of σ_{AA} for a few ϵ_{AB} . Since a small ϵ_{AB} leads to the weak interaction between the cluster and surface, and lowers the vibrational coupling between the cluster and the surface, it is easy to understand that the smaller ϵ_{AB} is the higher T_c is. A larger σ_{AA} also

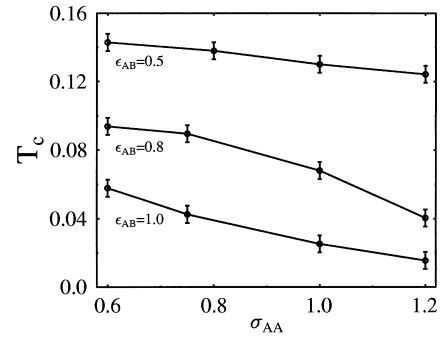


Fig. 5. The critical temperature T_c as a function of σ_{AA} for several ϵ_{AB} . The cluster with smaller σ_{AA} tends to be stable on surfaces with higher temperatures.

results in the greater interaction between the cluster and the surface, which is why T_c increases with the decrease of σ_{AA} for the same ϵ_{AB} . Additionally, the cluster with smaller atoms (small σ_{AA}) is more *hard* than that with larger atoms, since the *bulk modulus* [47] of the cluster is proportional to $1/\sigma_{AA}^3$. This may be another reason for the higher T_c values with larger σ_{AA} values.

Comparing our previous study about the cluster on the fcc(100) surface [15], we find that T_c for the cluster on fcc(100) surface is much lower than that on the fcc(111) surface. This is understandable since the cluster on the fcc(100) surface has a stronger interaction than that for the cluster on the fcc(111) surface for the same ϵ_{AB} .

3.3. Diffusion of the cluster on the surface

To study the diffusive behavior of the cluster on the surface, we choose $\epsilon_{AB}=0.5$ and $\sigma_{AA}=0.6$ – 1.4 . The simulations are carried out at $T=0.12$. At $T < T_c$ running after 2×10^5 steps, the structure of the cluster remains unchanged and does not wet on the surface. Visual observation shows that the diffusion inside the cluster or on the cluster surface is inhibited at this temperature. These results suggest that the cluster diffuses as a whole rather than by a single atom jump or dislocation mechanism.

Fig. 6 shows the obtained diffusion constants changing with σ_{AA} , in which the dashed line indicates the diffusion constant of an adatom on the surface with $\epsilon_{AB}=0.5$ at $T=0.12$. From the figure,

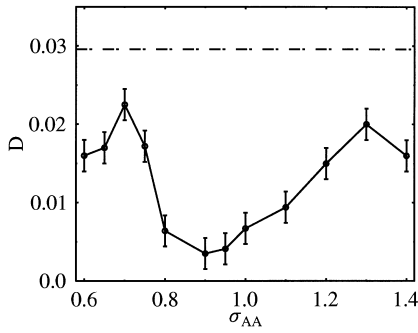


Fig. 6. Dependence of the diffusion constants on σ_{AA} ($\epsilon_{AB}=0.5$, $T=0.12$), the dashed line denotes the diffusion constant of an adatom at same temperature. The diffusion constant of the cluster is comparable with that for an adatom, and is strongly dependent on σ_{AA} .

we can see that, the diffusion of the cluster is very fast, and is comparable to that of an adatom. The diffusion constant reaches a minimum ca. $\sigma_{AA}=1.0$, and reaches a maxima symmetrically on both sides ca. 1.0, but the diffusion constants are not exactly the same on both sides. Different from previous results [42], the cluster with atoms smaller than the surface atoms tends to move more quickly.

The interface stress between the cluster and surface is the key to understanding the dependence of diffusion constants on σ_{AA} . As we have discussed in Section 3, wherever σ_{AA} deviates from 1.0, the mismatch between the cluster and the surface will increase. As the mismatch occurs there must exist stress between the cluster and surface. The stress will reduce the binding between the cluster and the surface comparing to the well-matched case ($\sigma_{AA}=1.0$) and correspondingly, the diffusion barrier will reduce. From Fig. 1, we can see that the high mismatch case is σ_{AA} ca. 0.7 and 1.3 ($\epsilon_{AB}=0.5$ only), and this is why the diffusion constant reaches the maxima ca. $\sigma_{AA}=0.7$ and 1.3, and reaches a minimum ca. $\sigma_{AA}=1.0$.

We find that the motion of the cluster in our case is dominantly due to the rolling of the cluster. We define $\Delta H = z_i - z_0$ as the height of a cluster atom relative to the mass center of the cluster, where z_i and z_0 are the coordinates normal to the surface for the cluster atom and mass center of the cluster, respectively. Fig. 7 shows ΔH changing with time step, the changes of ΔH from negative

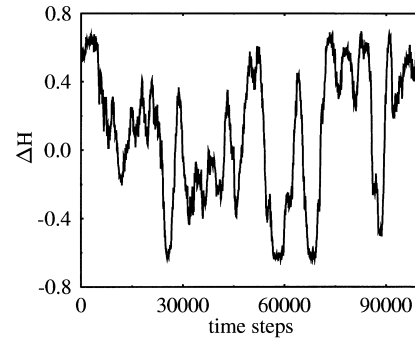


Fig. 7. ΔH the height to the center of the cluster for one cluster atom in MD runs. The changes of height from negative to positive imply the rolling of the cluster.

to positive suggest the cluster is rolling. If the cluster translates or rotates on the surface, the height should almost remain constant. To further illustrate the rolling process, Fig. 8 shows a snapshot of the rolling processor. The changes of the atom position relative to the surface (see the white atoms, for example) indicates the rolling of the cluster. If the cluster diffuses by translation or rotation, this triangle of the white atoms should be parallel to the surface at all times. To our knowledge, this new mechanism presented for

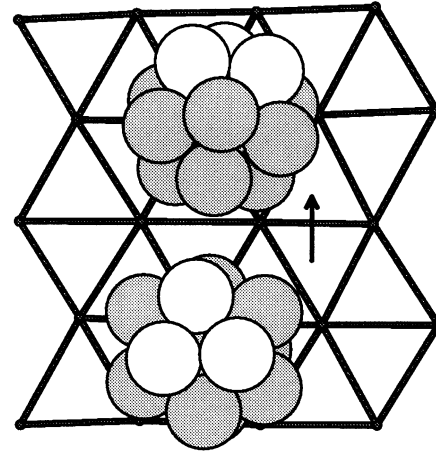


Fig. 8. A snapshot of the rolling process. The arrow indicates the diffusion direction. The distance between the clusters has been displaced to make the process more clear. The changes of the atom position relative to the surface (see the white atoms, for example) indicates the rolling of the cluster. If the cluster diffuses by translation or rotation, this triangle of white atoms should be parallel to the surface at all time.

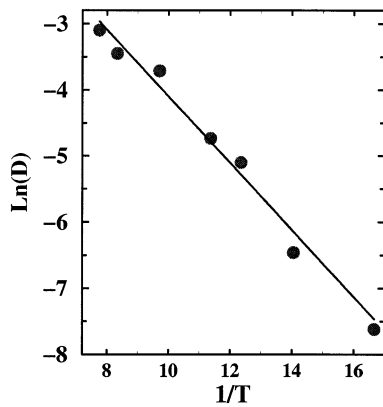


Fig. 9. Temperature dependence of the diffusion constant. The diffusion follows the Arrhenius law.

three-dimensional cluster on the surface has not been reported previously. This could be important for the understanding of the initial process of thin film growth. More important, the diffusion mechanism is weakly independent on the details of interatomic potential. In a recent study, the similar diffusion behavior has been observed by using more realistic potential [48].

It is interesting to look into the process of cluster rolling. When the rolling occurs, one atom in the bottom triangle face of the cluster rises, and at the same time another atom in neighboring triangle face falls onto the interface. During this process, the shared edge of the two triangle faces keeps unmoved. Consequently, the change of the interaction energy between the cluster and the surface during the rolling process is mainly related to the two atoms, the raised one must overcome a potential barrier, but the fallen one can have an energy gain. Compared to the cluster translation on the surface, where the three bottom atoms need to overcome the potential barrier simultaneously, the potential barrier for rolling is only ca. one-third smaller than that for translation. The small potential barrier for the cluster rolling could be the reason for the large diffusion constant which is comparable for the adatom.

We have studied the temperature dependence of diffusion constant for fixed values of σ_{AA} (0.7) and ϵ_{AB} (0.5), the obtained results can be fitted by the Arrhenius law (Fig. 9), with an activation

energy of 0.43 and a prefactor D_0 of 0.066. The obtained activation energy is only slightly larger than that for adatom (~ 0.28 , $\epsilon_{AB}=1.0$ and $\sigma_{AA}=1.0$).

4. Summary

In this paper, we have studied the structure, thermal stability and diffusion of a highly symmetric cluster on fcc(111) surface. We find that the surface tends to deform the structure of the supported cluster, however, the cluster can easily be stable on the surface without losing its structural characters with different ϵ_{AB} and large structural mismatch. The relationship between the stability of the cluster and the surface properties is obtained. We find that the supported cluster is only stable under a certain temperature T_c , which is much lower than the melting point of the free cluster. The dependence of T_c on σ_{AA} and ϵ_{AB} is also obtained. Instead of a single atom jump and dislocation mechanism, we find that the cluster can move very fast as a whole on the surface and the fast diffusion is dominantly due to the rolling of the cluster, which has a small activation energy. The close relationship between the diffusion constants and σ_{AA} is also obtained.

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