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Local Acceleration Effects of Adatom at the vicinity on the Surface: Case of Co Nano Thin-Films on Al Surface

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Abstract. The local acceleration effects, which are peculiar phenomena during atomic scale deposition process, were investigated by Molecular Dynamics (MD) simulation. The values of local acceleration were distributed widely for various surface orientations. Deposited atoms were accelerated along the potential energy surface, and accelerated values were evidently dependent on the local configuration of the surface. In contrast, the local acceleration became negligibly small for clusters consisting of many atoms.

Introduction

With the rapid development of nano device, understanding atomic scale phenomena become very important in manufacturing suitable device. Only 1 or 2 layer of intermixing occurred at the interface has affected on the performance of the devices. Recently, computational approaches based on reasonable theories have become helpful tools to understand such atomic scale phenomena since experimental approaches are not only inefficient but also methodologically not feasible. Especially, various approaches using molecular dynamics (MD) helps us to rationalize many kinds of thin film growth behaviors which are not easy to observe from experimental approaches. For example, depositing atoms with low incident energy can be deflected toward three-dimensional surface, a so-called "steering effect", results in a rougher surface [1]. In connection with this steering effect, "local acceleration effect" was observed when adatoms obtain sufficiently large value of acceleration energy regardless of its initial incident energy at the vicinity of surface [2, 3]. In the investigations of deposition behaviors in Co-Al system using molecular dynamics method, It is reported that Co adatom was intermixed with surface Al atoms regardless of Al substrate orientations in spite of 0.1 eV of low incident energy and it is originated from relatively low energy barrier for incorporation process [4, 5]. In this study, we investigated systematically and quantitatively the phenomenon of deposited atoms being accelerated at the vicinity of the surface, namely, "the local acceleration", focusing on the case of the Co-Al system.

Calculation Procedure

Interatomic potentials were based on the Embedded Atom Method (EAM), which is well known for metallic system [6], and Voter and Chen potentials for Al-Al, and Passianot and Savino potentials for Co-Co were adapted to the XMD 2.5.32 code [7, 8, 9, 10]. The cut-off distance for Co, Al, and Co-Al was set to 5.26 $\mathring{A}$, 5.55 $\mathring{A}$, and 5.6 $\mathring{A}$, respectively. The employed EAM potentials are in

good agreement with the experimental results for pure elements and the intermetallic compounds between constituent metal atoms. For molecular dynamics simulation, sufficiently large (001), (011) and (111) Al surfaces were prepared and the z-direction was set normal to the each orientations. Periodic boundary conditions were utilized in the x and y-directions. To minimize the errors from the thermal vibration, substrate temperature was kept at 0 K using Nosé-Hoover thermostat method. The differences between initial kinetic energy and the maximum detected kinetic energy were recorded as a local acceleration value for the condition. The incident energy of adatom was set to 0.1 eV and the adatom was added 10 $\AA$ from the substrate surface, which is farther than the cut-off distance. The incident angles were set normal to the substrate.

Results and Discussions

Figure 1 shows a local acceleration contour with respect to the incident position of Co adatom on Al(001), (011) and (111) surfaces. Each line represents the same value of the local acceleration. In Fig. 1 (a), the local acceleration on hollow site shows the maximum value and on top site corresponds to the minimum. Hollow site is energetically less stable than on top site. Similarly, concave sites on (011) and (111) surfaces show higher acceleration tendency. The degree of acceleration depends on the coordination numbers of surface neighbor-atoms when adatom approaches to the surface. This is directly related to the surface morphology. Also, the local acceleration is proportional to surface instability. Therefore, the acquired local acceleration distribution have the same characteristics as potential energy surface (PES). At the center of (011) surface (Fig. 1 (b)), the highest acceleration is shown since (011) surface is very unstable and, consequently, can be easily influenced by attractive force from surface atoms. On (111) surface(Fig. 1(c)), local acceleration distribution followed the surface configuration and the variation of the values was relatively small, resulting from the fact that (111) surface is the densest of all surfaces.

For further insights of local acceleration characteristics of each surface, the range of local acceleration, the average value, and mixing ratio was compared in Table 1. It is relevant to note that the maximum value at local acceleration was 3.8 eV for (001), 4.2 eV for (011), and 3.5 eV for (111) since the value is directly related to the surface instability. The range of local acceleration for (111) surface was relatively narrow, and (011) surface shows relatively wide distribution. This observation agrees

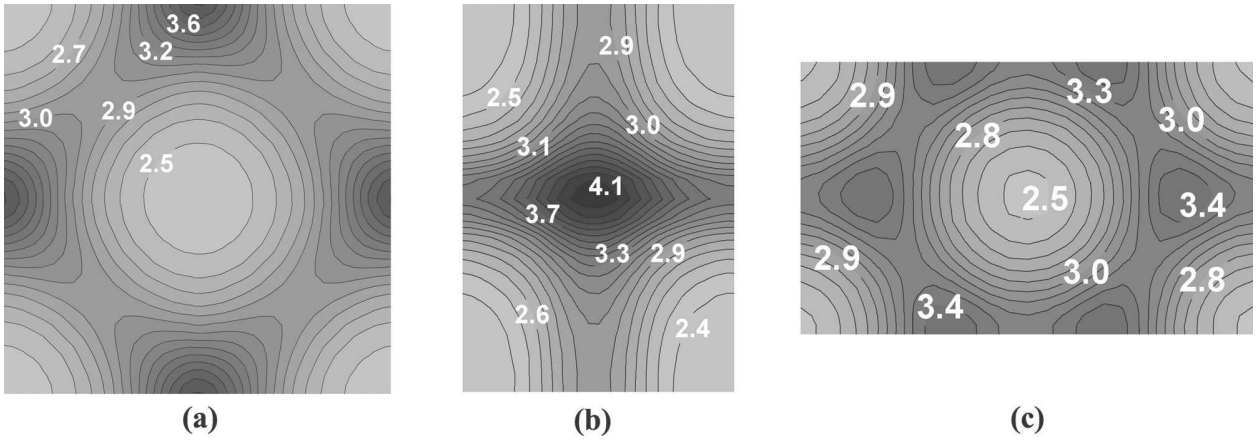

Fig. 1: The local acceleration contours of Co adatoms on for each Al surface orientations: (a) Co on Al(001), (b) Co on Al(011) and (c) Co on Al(111). Each line is separated by 0.1 eV intervals from 2.4 to 4.1 eV, and degree of the local acceleration is proportional to darkness of contour.

Surface orientations	Range (eV)	Average (eV)	Mixing Ratio (%)[a]
(001)	2.4 ∼ 3.8	2.89	90
(011)	2.2 ∼ 4.2	2.85	56
(111)	2.5 ∼ 3.5	3.01	82

[a]Ref. 4.

Table 1: Distributions of the local acceleration values, average and mixing ratio for the case of Co on Al substrate with each surface orientations.

well with the atomic density data for each surface. In contrast, the average value of local acceleration was highest for (111) surface and lowest for (011). The average value of local acceleration is very critical to understand the surface alloying or mixing because the local acceleration was considered to be a key factor for surface alloying observed in Co-Al system [4]. In our previous work, the highest mixing ratio was found in Al(001), and the lowest mixing ratio in Al(011), as summarized in Table 1. It is believed that the mixing rate for Co on Al(001) surface could be enhanced due to less than 0.1% of lattice mismatch between Al(001) and CoAl(001) and, naturally, highly ordered B2 structure was formed on Al(001) surface. It is worth mentioning that the structures of the surface alloy on (011) and (111) surfaces were found to be amorphous.

Most researches related to the local acceleration were centered on the case of 1 atom deposition process. In an attempt to investigate the effect of size of cluster on the local acceleration, the deposition simulation of the various size of clusters consisting of Co atoms on Al(001) surface was performed. (Fig. 2) As shown in Fig. 2, the value of the local acceleration rapidly decreased as the number of atoms of cluster increased. In the case of cluster of about 400 atoms, corresponding to merely 2.2 nm in diameter, the degree of acceleration for the cluster was found to be minimal. Since the attractive force of the surface Al atoms reaches only to about 5 $\AA$ from the surface, it would be reasonably concluded that the large size cluster could not be easily accelerated.

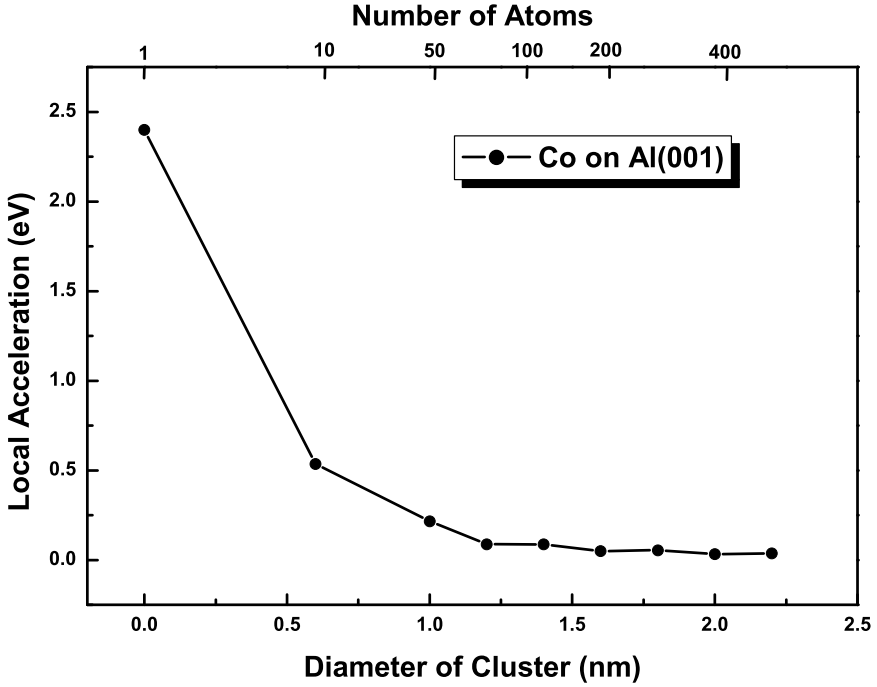

Fig. 2: Local acceleration as a function of cluster size and number of atoms for Co on Al(001).

Conclusions

Using a molecular dynamics simulation, the local acceleration which is one of the key factor for the surface intermixing found in Co-Al system was quantitatively investigated. The acceleration was shown to be largely proportional to the attractive force of surface atoms. Especially, the (111) surface showed the highest acceleration on average than any other surfaces, (001) and (011), and (011) surface corresponds to the widest distribution. This kind of local acceleration is the characteristics of atomic scale deposition. In case of cluster deposition, the local acceleration value rapidly decreased and became a negligibly small for clusters larger than 2.0 nm in diameter. It is expected that the understanding this observation help to rationalize the fundamental reasons for serious problems such as "steering effect" in thin film growth processing, and offer very helpful guidelines upon the phenomena that intermixing layer is spontaneously formed in spite of low incident energy of adatom.

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