

Asymmetric surface intermixing during thin-film growth in the Co–Al system: Role of local acceleration of the deposited atoms

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Received 27 April 2007; received in revised form 30 October 2007; accepted 31 October 2007

Available online 21 December 2007

Abstract

Surface intermixing behavior during thin-film deposition in the Co–Al system was investigated on the atomic scale by three-dimensional classical molecular dynamics simulation. Asymmetry of the surface intermixing was observed: Al deposition on a Co substrate resulted in an Al thin-film with an atomically sharp interface, while a Co thin-film deposited on an Al substrate had an interfacial intermixing layer of B2 structure. This phenomenon is discussed in terms of the kinetics of atomic intermixing on the surface. A kinetic criterion for the atomic intermixing is whether the increased kinetic energy of the deposited atom near the surface is larger than the energy barrier to atomic intermixing on the surface. Local acceleration of the deposited atoms near the surface provides an explanation of the puzzling phenomenon of the significant intermixing under low-energy deposition conditions such as thermal evaporation or molecular beam epitaxy.

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Keywords: Multilayer thin-films; Deposition; Interface structure; MD simulation

1. Introduction

Thin multilayer structures are widely used in current devices and sensors, such as spintronics devices utilizing the tunneling magnetoresistance or the giant magnetoresistance phenomena [1]. Because of the short coherence length of spin polarization, electric spin phenomena can only occur across a thickness of a few nanometers in ordered thin-films [2,3]. Thin-films or multilayers less than 1 nm thick are thus extensively used in these devices. The electromagnetic phenomena in these multilayer systems are largely dependent on the interface structure between thin ferromagnetic and nonmagnetic layers [4–7]. It is further noted that the interface structure limits diffusive electrical spin injection efficiency across a heteroepitaxial interface [2]. Therefore, atomic scale control of the interfacial structure is one of the major issues in developing these devices,

and requires an in-depth understanding of the surface reaction during thin-film deposition.

Atomic scale intermixing behavior on surfaces has drawn much attention since the 1990s and surface analysis tools such as the scanning probe microscope have been widely used. Rousset et al. [8] investigated the deposition of Au atoms on the Ag(110) surface to address the surface alloying effects on the thin-film growth mode, whereas earlier growth models [9], such as the Volmer–Weber, Frank–van der Merwe or Stranski–Krastanov growth models, had treated the substrate as an inert template. Rousset et al. reported that the Au grows in a layer-by-layer mode on the Ag(111) and (100) surfaces, whereas significant surface intermixing was observed on the Ag(110) surface [8]. Chan et al. [10] reported the possibility of surface intermixing when Au atoms are deposited on the Ag(110) surface using first-principles calculation. He and Wang also observed surface intermixing in Au–Fe systems and considered the growth phenomenon with interfacial intermixing as a new growth mode [11]. Similar observations of surface

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intermixing during the initial stage of thin-film growth have been reported for Ag–Al [12], Fe–Cr [13], Fe–Cu [14] and Co–Al [7].

Asymmetry of atomic intermixing on the surface has been observed in some thin-film systems. Buchanan et al. [15,16] extensively studied the interfacial intermixing behavior in Al–*X* multilayers, where *X* represents transition metals from rows 4, 5, and 6 of the Periodic Table. They observed that the intermixing was considerably less when Al was sputtered onto the metal *X* than when *X* was deposited on Al, resulting in an asymmetric interfacial structure. Although they could not suggest a complete model to account for the experimental observations, they reported that the only correlation found between the intermixing length and bulk parameters was between the cohesive energy of the substrate materials and the intermixing length. The asymmetry of the surface intermixing has been observed in a wide range of metallic thin-film systems, such as Au–Ge [17], Au–Ni [18], Co–Al [5], Cu–Ni [19,20], Fe–Cr [13] and Co–Cu [6].

Thin-film growth usually occurs far away from thermodynamic equilibrium conditions [21]. Even if the intermixing between atoms is energetically favorable, the atomic exchange process leading to surface intermixing is characterized by a finite value of the energy barrier to the exchange. The kinetic constraints that prevent the deposited atoms from reaching their thermodynamically optimum position are more significant at low temperature [22]. The details of the deposition kinetics and the formation of the nonequilibrium complicated structures can be addressed by molecular dynamics (MD) simulations. HafTEL et al. [23,24] investigated the deposition behavior in Au–Ag and Au–Pt systems by empirical MD simulation, and observed the asymmetry of the intermixing in the Au–Pt system. Zhou et al. [25] reported the asymmetry of the interfacial structure in the Ni–Cu system by MD simulation of thin-film deposition at room temperature. They considered the energy barrier to the atomic exchange in efforts to understand the asymmetric intermixing behavior. They showed that significant intermixing occurs only on the substrate surface of the smaller energy barrier to the atomic exchange. However, the calculated energy barrier to the intermixing appeared to be larger than the kinetic energy of the deposited atom, even when significant intermixing was observed. Zhou et al. had to introduce a non-perfect form of the surface that has a very low-energy barrier to the exchange to explain this puzzling phenomenon.

In the present study the authors investigated the interfacial structure in the Co–Al thin-film system at room temperature by using empirical MD simulation. Co and Al exhibit almost no solubility with each other at room temperature, while many intermetallic phases of Al_xCo_y , including the stable AlCo intermetallic phase of B2 structure, exist [26]. Hence, intermixing between these elements will not result in a solid solution but rather in an intermetallic phase. Atomic scale deposition behaviors were simu-

lated with a perfect single-crystalline substrate and with the initial kinetic energy of the deposited atoms fixed at 0.1 eV. Even under these conditions asymmetric interfacial intermixing was observed: Co deposition on the Al substrate resulted in significant surface intermixing, while the Al thin-film grows on the Co with an atomically sharp interface. As in the Ni–Cu case [25], the energy barrier to the intermixing on the Al surface is much larger than the initial kinetic energy of the deposited Co atom. In the present study, we focused on a rapid increase in the kinetic energy of the deposited atoms near the substrate surface because of the chemical attraction between atoms. We showed that the local acceleration of the deposited atoms can induce surface intermixing even if the energy barrier to the intermixing is larger than the initial kinetic energy of the deposited atoms.

2. Calculation methods

Semi-empirical embedded atomic method (EAM) potentials developed by Pasianot and Savino for Co–Co [27], Voter and Chen for Al–Al [28], and Vaillhé and Farkas for Co–Al [29] were used to simulate the deposition behavior in the Co–Al system at 300 K. The potentials used in this study were rigorously benchmarked by using the calculated or experimentally observed lattice constants, mechanical properties, surface energies and thermodynamic stability of the phases. Table 1 summarizes the benchmark test of the potentials used in this study. Lattice constants, cohesive energy and elastic constants exhibit quantitative consistency between molecular static calculations and experiments or the first-principles density functional theory (DFT) calculations. The qualitative relationship between the surfaces is in good agreement with the DFT calculations. For example, the calculated surface energy of Co is larger than that of Al, as in the DFT calculations, although the surface energy of Co is underestimated for all orientations. In the present study, the cutoff distances for Co, Al, and Co–Al were set to 5.26, 5.55 and 5.6 Å, respectively.

The single crystal substrate of the face-centered cubic (fcc) structure was set to $16a_0 \times 16a_0 \times 6a_0$, where a_0 is the bulk lattice constant of each respective element. No defects or steps were artificially introduced into the substrate surface. The total number of the substrate atoms was 6144. Although the equilibrium structure of Co at 300 K is hexagonal close packed (hcp), fcc Co substrate was used in the present simulation because the fcc structure is frequently observed in Co thin-films [30]. Furthermore, it should be noted that the energy difference between the two closely packed phases (fcc and hcp) of Co is very small [37,40]. A periodic boundary condition was adopted in the lateral directions. The atomic position of the bottom-most layer was fixed to simulate a thick substrate. Temperature of the bottom three layers was fixed at 300 K so that the layers acted as a thermal bath during deposition. All the other atoms were unconstrained. The substrate was equilibrated with a thermal bath for 5–10 ps by the MD

Table 1
Summary of the benchmark test for the potentials used in this study

Property	Co				CoAl		Al	
	Exp. or DFT	Calc.	Exp. or DFT	Calc.	Exp. or DFT	Calc.	Exp. or DFT	Calc.
Structure	A3 (hcp)		A1 (fcc)		B2		A1 (fcc)	
a_0 (Å)	2.51[37]	2.507	3.55[40]	3.545	2.86[42]	2.86	4.05[37]	4.05
E_{coh} (eV)	4.39[37]	4.39	4.38[40]	4.383	4.45[43]	4.47	3.36[37]	3.37
C_{11} (GPa)	307.1[38]	319	238[41]	242.7	268.8[44]	225.6	114[38]	107
C_{12} (GPa)	165[38]	166	158[41]	167.3	107.2[44]	145.6	61.9[38]	65.2
C_{13} (GPa)	102.7[38]	101.9	–	–	–	–	–	–
C_{33} (GPa)	358.1[38]	373.1	–	–	–	–	–	–
C_{44} [GPa]	75[40]	82.3	128[41]	146.7	139.2[44]	115.2	31.6[38]	32.2
γ_{111} (mJ/m ²)	–	–	2700[45]	1000	–	1863	935[39]	831
γ_{100} (mJ m ⁻²)	–	–	2800[45]	1196	–	1799	1081[39]	869
γ_{110} (mJ m ⁻²)	–	–	–	1364	–	1574	1090[39]	1006
γ_{0001} (mJ m ⁻²)	2775[39]	1013	–	–	–	–	–	–
γ_{1010A} (mJ m ⁻²)	3035[39]	1118	–	–	–	–	–	–
γ_{1010B} (mJ m ⁻²)	3791[39]	1372	–	–	–	–	–	–

relaxation of the structure. Atoms were then deposited in a direction normal to the surface. The kinetic energy of the deposited atoms was set to 0.1 eV, which is typical of that found in evaporation or molecular beam epitaxial growth. The positions of the deposited atoms were randomly selected. The deposited atoms were added at a distance of 16.8 Å from the substrate surface. The time step for the MD simulation was 0.1 fs to obtain accurate atomic trajectories. The time interval between two consecutive depositions on the substrate was fixed at 5.5 ps. The temperature of the substrate was rescaled to 300 K after the atomic rearrangement caused by the bombardment of the deposited atom had settled down.

3. Results and discussion

Asymmetric surface intermixing occurs during the early stage of thin-film growth in the Co–Al system. Fig. 1a shows the surface structure when one monolayer (ML) of Al atoms was deposited on the Co(001) surface. The gray and dark gray spheres represent the Al and Co atoms, respectively. The surface structure shows that the Al monolayer is deposited on the Co surface with an atomically sharp interface. The sharp interface is maintained during further deposition of Al. Fig. 1b is a snapshot of a specimen after 1536 Al atoms had been deposited on the Co substrate. Fig. 1c shows the composition variation across the interface, revealing the sharp interface on an atomic scale. On the other hand, severe surface intermixing occurs when Co atoms are deposited on the Al(001) surface. Fig. 1d is the snapshot of MD simulation when one ML of Co atoms was deposited on the Al substrate. In contrast to Fig. 1a, atomic exchange occurs between the deposited Co atoms and the substrate Al atoms, resulting in a subsurface Co layer, as indicated by an arrow. Subsurface Co atoms are located on the substitutional site, causing the substrate Al atoms to protrude from the surface. More details will be discussed in Fig. 3. After forming the subsurface layer, a thin-film of pure Co grew on the intermixed

layer, as can be seen in the snapshot of the specimen after 4096 Co atoms had been deposited (Fig. 1e). The compositional change across the interface of Fig. 1f clearly shows the surface intermixing.

The radial distribution function (RDF) of the intermixed region of Fig. 1e was compared with those of the fcc Al and CoAl B2 phases in Fig. 2. The RDF peaks of the intermixed layer are considerably smeared because of the defects and/or displacement of atoms from the lattice point. However, it is evident that the intermixed region has the characteristics of the CoAl B2 phase. Intermixed region and fcc Al substrate has an orientation relationship of fcc $\langle 100 \rangle \parallel$ B2 $\langle 110 \rangle$. We also measured the vertical and the lateral distance between atomic layers of the intermixed region. The vertical distance is 1.43 Å and the lateral distance along the fcc $\langle 100 \rangle$ direction 2.03 Å. Because the B2 structure is rotated by 45°, the lattice parameter a is $2.03/\sqrt{2} = 1.428$ Å. The c/a ratio of the intermixed region is about 1, which confirms the cubic B2 structure. This result shows that most of the deposited Co atoms exchange surface Al atoms to form an interfacial layer of B2 structure. The characteristics of fcc Al remain in the RDF spectrum because the selected intermixed region for the RDF characterization includes a pure Al layer on the bottom. A similar deposition behavior, characterized by the asymmetric interfacial structure, was also observed on the (111) and (110) substrate surfaces. However, an amorphous mixing layer was observed when Co was deposited on the Al (111) and (110) substrates [46].

The asymmetric intermixing behavior in the Co–Al system was experimentally confirmed by coaxial impact collision ion-scattering spectroscopy [31] and by measuring the magneto-optical Kerr effect of the Co–Al thin-film system [32]. Shivaparan et al. [5] and Buchanan et al. [15,16] also reported experimental results supporting the asymmetric surface reaction in the Co–Al system. The asymmetry cannot be explained by the thermodynamic stability of the phases involved because the thermodynamic stability should result in a symmetric interfacial structure. The

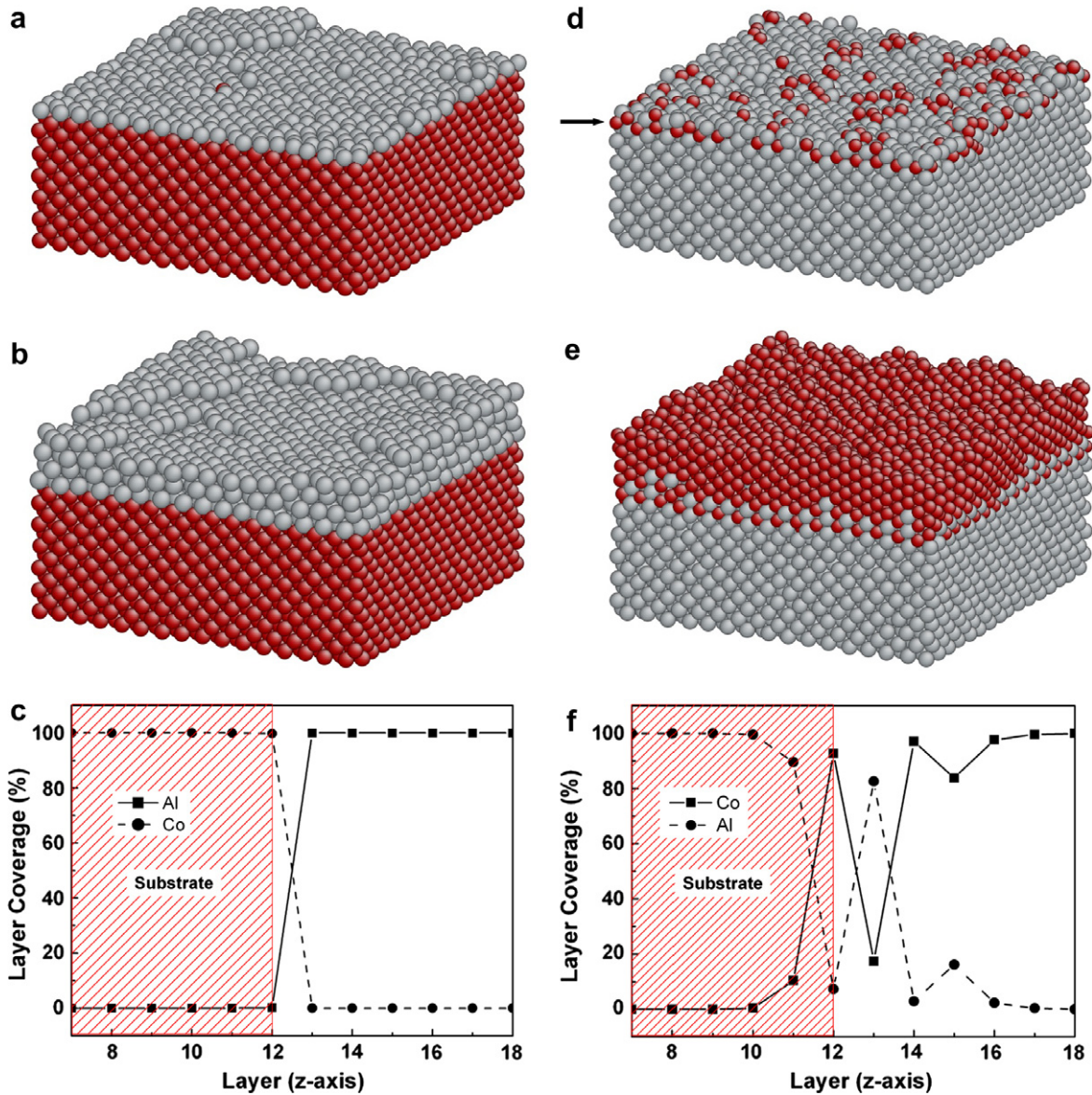


Fig. 1. Snapshots of the simulated surface of (a) one monolayer of Al deposition on Co(001) and (b) 1536 Al atoms deposited on the Co(001) surface with (c) the composition variation across the interface. Snapshots of the simulated surface for (d) one monolayer of Co deposition on Al(001) and (e) 4096 Co atoms deposited on the Al(001) surface with (f) the composition variation across the interface.

difference in surface energy between the deposited and substrate elements can be considered to govern the exchange behavior on the substrate surface [9]. The surface energy criteria suggest that if the surface energy of the deposited element is larger than the sum of the surface energy of the substrate element and the interfacial energy between deposited and substrate elements, deposited atoms will penetrate into the substrate to minimize the total energy of the system. This process might be important at high substrate temperatures where the thermally activated atomic process is significant. However, the thermally activated process is considerably restricted at room temperature and hence the surface segregation cannot fully account for the asymmetry observed in the present study that simulates the deposition behavior at 300 K. In addition, it

must be noted that the intermixing is highly limited in the interfacial region, as shown in Fig. 1e and f. If the atomic exchange is governed by the surface energy criteria, then long-range distribution of Al in Co thin films will be observed because the driving force for the diffusion of Al to the surface will remain throughout the entire deposition process. It is thus evident that the deposition processes in the present study are highly constrained by the kinetic criteria.

Another observation supporting the importance of the kinetic criteria is the sequential snapshots of single Co atom deposition on the Al(001) surface that reveals the details of the atomic process of the deposition (Fig. 3). A Co atom approaches the substrate (Fig. 3a) at 0.35 ps after starting the simulation and dynamically penetrates along

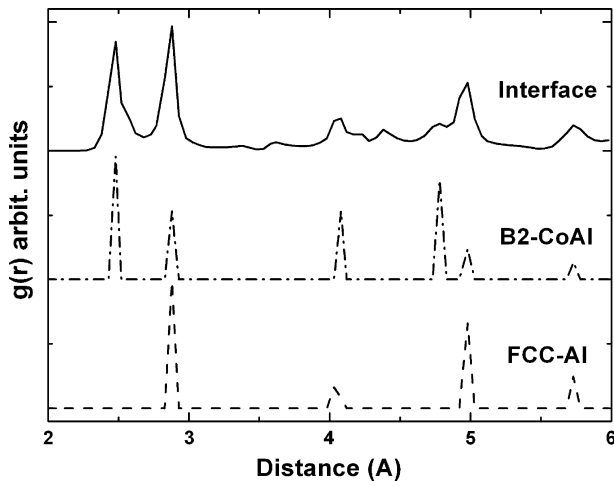


Fig. 2. Radial distribution functions of the intermixed region of Fig. 1e, CoAl B2 structure and fcc Al structure.

the interstitial path to the subsurface interstitial site (see Fig. 3b–e). The Co atom then pushes the Al atom upward from the surface as it moves to the substitutional site (Fig. 3f). Because the diameter of the Co atom is smaller than that of Al, the Co position is not coincident with that of substrate Al. The entire process of atomic exchange on the surface occurs within about 1 ps of the deposited Co atom arriving on the Al surface. The dynamic penetration is in contrast to the previous understanding of atomic exchange, where the deposited atoms land on the surface and are then subjected to exchange with the substrate atoms depending on thermodynamic criteria such as total energy minimization [23]. Because thermally activated atomic hopping or diffusion is involved in the exchange process, there can be a time delay between the exchange event and the moment when the deposited atom attaches to the surface. However, Fig. 3 shows that the arrived

atoms dynamically penetrate into the substrate without staying on the surface.

The present MD simulation implies that the surface intermixing behavior should be understood in terms of the kinetic criteria, such as the energy barrier of the atomic intermixing reaction, as was suggested by Zhou et al. [20,25]. Using a molecular static calculation, the energy barrier to the deposited atoms penetrating the (100) substrate surface on the hollow site was calculated. Two extreme cases were considered in this calculation, namely an energy barrier with and without relaxation of the substrate atoms during penetration. In the former case, the local equilibrium is maintained during the penetration process, and in the latter the substrate atoms cannot respond at all to the penetration of the deposited atoms. In an actual penetration process the energy barrier will be between these two extreme values, depending on the rigidity of the substrate atoms and the deposition conditions, such as the kinetic energy of the deposited atoms or the deposition temperature. For example, a rigid substrate will be more resistant to relaxation during penetration. If the deposited atoms bombard the substrate at very high velocity, then the substrate atoms cannot undergo relaxation.

Table 2 summarizes the calculated energy barriers for the penetration. When Co atoms are deposited on the Al(001) surface the energy barrier will be between 4.78 eV for fixed substrate atoms and 0.56 eV for full relaxation. Similarly, the energy barrier required for the Al atoms to penetrate into the Co(001) surface is between

Table 2
Energy barrier to atomic penetration (eV)

	Without relaxation	With relaxation	Median value
Co on Al(001)	4.78	0.56	2.67
Al on Co(001)	5.95	1.66	3.81

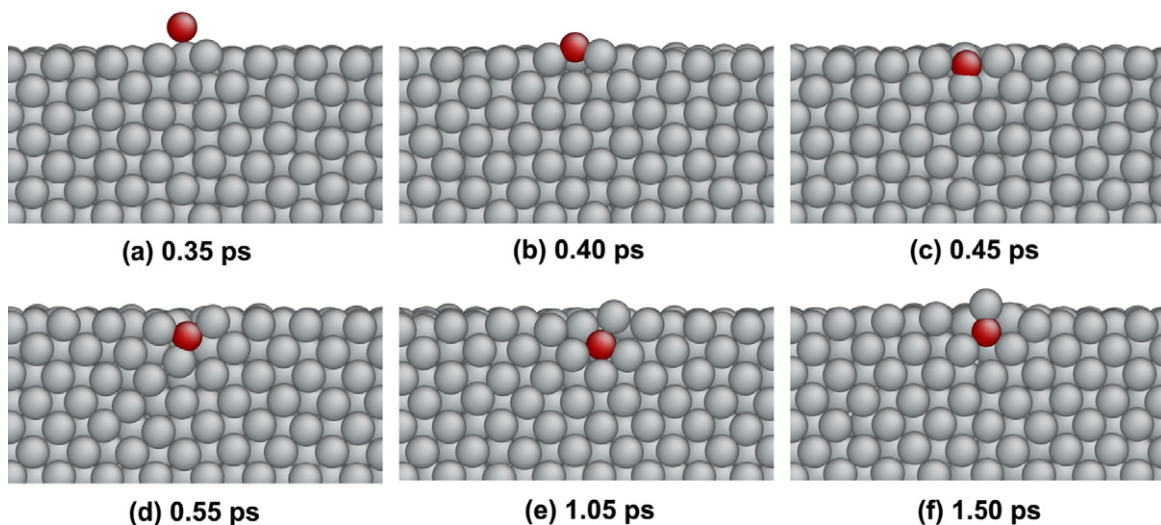


Fig. 3. Sequential snapshots of single Co atom deposition on the hollow site of the Al(001) surface.

5.95 and 1.66 eV. Kim et al. estimated the energy barriers to atomic penetration in the Co–Al system by a first-principles calculation based on DFT calculations [33]. The energy barrier to penetration of deposited Co atoms into the Al(001) substrate is 0.39 eV, while that for the Al atoms into the Co(001) substrate is 1.28 eV. These values are in good agreement with the present results obtained in the case of full relaxation of the substrate atoms. Because Al is softer than Co, the energy barrier on the Al substrate will be closer to the relaxed value than that on the Co substrate. However, if we simply assume that the effective energy barrier is the median of the two extreme values, then the energy barriers will be 2.67 and 3.81 eV, respectively. The asymmetry of the interfacial intermixing would be a consequence of this large difference in the energy barriers of atomic intermixing, i.e. the kinetic probability of the atomic penetration to the substrate.

However, it should be noted that the effective energy barrier to penetration of the Co atom into the Al substrate (about 2.67 eV) is much larger than the initial kinetic energy of the Co, 0.1 eV. Because thermal energy at room temperature is about 0.02 eV, it can hardly be expected that thermal vibration can supply sufficient kinetic energy to overcome the energy barrier. A similar discrepancy in the quantitative analysis of the interfacial reaction exists in the Cu–Ni system investigated by Zhou and Wadley [25]. To address the discrepancy, we observed the kinetic energy of the deposited atom during deposition. Fig. 4 shows the energy change of the deposited Co atom when deposited on the hollow site of the Al(001) surface. Letters on the kinetic energy curve indicate the energies associated with the snapshots of Fig. 3. The initial kinetic energy of the deposited atom is 0.1 eV with zero potential energy. (The potential energy of an infinitely separated atomic configuration was chosen as the reference state.) As the deposited atom approaches the substrate, the kinetic energy increases very rapidly in the vicinity of the substrate surface. This

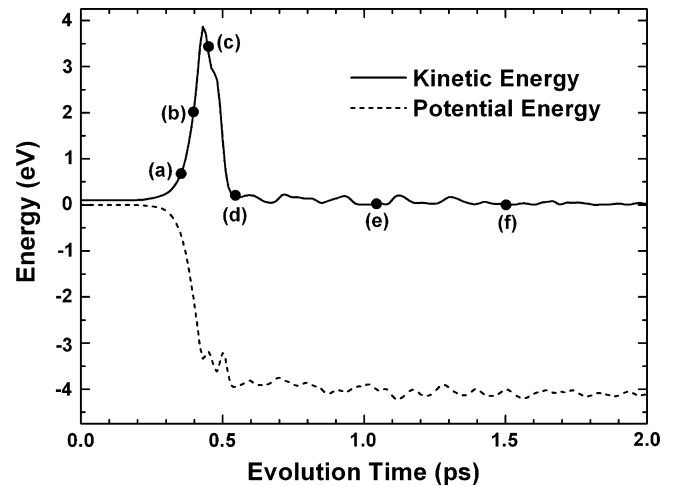


Fig. 4. Time evolution of the kinetic and potential energy of the deposited Co atom on the hollow site of the Al(001) surface.

increase in the kinetic energy or acceleration to the substrate is accompanied by a rapid decrease in the potential energy. The local acceleration near the substrate is natural in most systems where the potential energy curve between the deposited atom and the substrate has a minimum at the equilibrium distance. The magnitude of the acceleration is proportional to the slope of the potential curve with respect to the atomic distance, i.e. the attracting force between the deposited atoms and the substrate atoms. The local acceleration has also been widely discussed in efforts to understand the steering phenomena during thin-film growth [34–36].

Because any substrate atom influences the potential surface of the deposited atom, the local acceleration is dependent on the deposition position on the substrate surface. Fig. 5 shows the maximum kinetic energy contour on the (001) substrate surface. The local acceleration is maximized when the deposited atoms approach the substrate

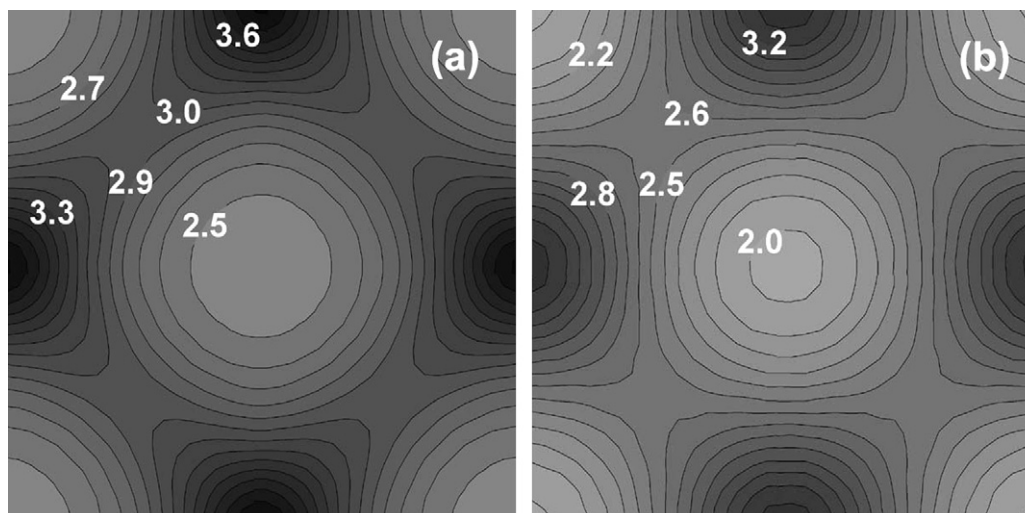


Fig. 5. Contour map of the maximum kinetic energy of (a) Co atoms deposited on Al(001) surface and (b) Al atoms deposited on the Co(001) surface.

on the hollow site (dark region), while it is minimized on the top of the substrate atoms (bright region). In the case of Co deposition on the Al(001) surface (see Fig. 5a) the maximum kinetic energy ranges from 2.16 to 3.84 eV. Because the median of the energy barrier to penetration of Co into the Al substrate is 2.67 eV it can be said that most Co atoms will overcome the energy barrier to penetration into the Al substrate if the Co atoms do not approach the top of Al atoms. Fig. 5b shows the local acceleration behavior when Al atoms are deposited on the Co(001) substrate. The maximum kinetic energy of the Al atoms accelerated by the substrate Co atoms ranges from 1.87 to 3.24 eV. These values are considerably smaller than the median value of the energy barrier to the Al atoms penetrating into Co (3.81 eV). Therefore, no Al atoms can penetrate into the Co substrate and this results in an atomically sharp interface.

4. Conclusions

The most significant result of this study shows that the asymmetry of the surface intermixing during thin-film growth can be understood by comparing the kinetic energy of the deposited atom in the vicinity of the substrate with the energy barrier preventing the deposited atom from penetrating into the substrate surface. The present simulation reveals that surface intermixing occurs by dynamic penetration of the deposited atoms into the substrate. Even if the energy barrier to atomic penetration into the perfect substrate is larger than the initial kinetic energy of the deposited atoms, the local acceleration of the deposited atom in the vicinity of the substrate surface can provide enough kinetic energy to overcome the energy barrier to atomic penetration. Surface intermixing occurs if the sum of the initial kinetic energy of the deposited atom and the local acceleration is larger than the energy barrier to surface intermixing.

Acknowledgement

This work was financially supported by the KIST core capability enhancement program, Contract Nos. 2V00910 and 2E19190.

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