MOLECULAR DYNAMICS SIMULATION OF THE INTERACTION BETWEEN CLUSTER BEAMS AND SOLID SURFACES

Hee Jae Kang, Min Wha Lee and Chung Nam Whang*

Department of Physics, Chungbuk National University, Cheongju 360-763, Korea

*Department of Physics, Yonsei University, Seoul 120-749, Korea

ABSTRACT

The mechanism of the ionized cluster beam deposition has been studied using Molecular Dynamics Simulation. The Embedded Atom Method(EAM) potential were used in the simulation. The impact of a Au_{95}-cluster on Au(100) substrate was studied for the impact energies 0.15-10eV/atom. The dependency of the impact energy of cluster beam was observed. For the cluster energy impact of 10eV per atom, the defects on surface were created and the cluster embedded into substrate as an amorphous state. For the energy of 0.5eV per atom, the defect free homoepitaxial growth was observed and atomic scale nucleation was formated, which are in good agreement with experiment. Thus molecular dynamics simulation is very useful to study the mechanism of the ionized cluster beam deposition.

1. INTRODUCTION

Recently, Ionized Cluster Beam Deposition(ICBD) method[1-5] have received much attention because of various applications such as semiconductor, metal, dielectric for micro electronic device, optical coatings, optoelectronic device, magnetic materials and organic materials. ICBD has unique merits compared with other thin film growth method such as thermal deposition, ion plating, chemical vapor deposition. The kinetic energy of cluster beam is controllable during film growth. It should enhance chemical reaction between thin film and substrate materials. Therefore high quality thin films can be obtained at low temperatures, and single crystal thin film can be obtained even if it has a large lattice mismatch between thin film and substrate materials[2]. It was found experimentally that the nucleation density, packing density, sticking coefficient and epitaxial growth strongly depend on the energetic cluster energy. The aim of this paper is to clarify the mechanism of thin film growth by ICBD and to find the energy dependency of single crystal growth using molecular dynamics(MD) calculation.

2. THE SIMULATION MODEL

The MD simulations in this work are fully dynamical, three dimensional calculations which were performed using a version of Sput93[6]. It was developed by Garrison group for the simulation of several keV particle bombardment(sputtering) of solid. We extended it for the simulation of the interaction between cluster beam and solid surface. The details of this program can be seen elsewhere[7]. A predictor-corrector is used to integrate the equations of motion which are second-order, linear differential equations. The Embedded Atom Method(EAM) potential[8,9] was employed for the interaction between Au cluster and Au substrate, which is an empirical many-body potential energy function used primarily for the description of the metals, e.q. , Ni, Cu, Ag, Pt, Au and their alloys. The Au(100) substrate has a dimension $24a_o \times 20a_o \times 24a_o$ for the energy of 10eV/atom and $12a_o \times 5a_o \times 12a_o$($a_o$ is lattice distance) for the energy of less then 2eV/atom, where y axis is surface plane. Periodic boundary conditions in two axis(x,z) of the Cartesian directions were employed. No constraints or damping were placed at the substrate surface (010) plane. The generalized Langevin Equation was used to take into account thermal vibration and substrate temperature fixed at 300K.

3. RESULTS AND DISCUSSION

The interaction between Au cluster of 95 atoms with kinetic energy of 10eV/atom and Au(100) substrate is shown as function of time in fig.1. Here the center of cluster was started at 5.62Å from sample surface as seen in fig.1(a). The time step was chosen to be 1fs. As the impact begins, the atoms in the cluster begin to compress substrate interface, at the same time cluster and substrate lose its crystalline structures. As the time elapses, cluster atoms are broken up and penetrate into substrate, that is intermixing layer formed. Fig. 2 shows the results of 2 eV/atom as function of time. After 300 femto second, the atoms of the cluster start colliding with the substrate atoms(fig.2(b)). After 3000 femto second, the cluster atoms are actively moving but not widely spread out Au substrate and became equilibrium state after about 20 pico second. To see, in more detail, the redistribution of cluster atoms on substrate, fig.2(d) was replotted as top view and side view(fig.4(a)). The filled circles indicate the surface atoms of the topmost atomic layer of Au(100), and open circles is the deposited cluster atoms. From the top view, the cluster atoms can be seen how to be distributed into or onto substrate. It is of interest to note that most atoms of cluster sit on or accomodate into substrate while maintaining lattice distance except a few atoms. But some of defects are still observed on the topmost atomic layer, and parts of cluster atoms penetrate into more than 3rd layer from the surface even

if their kinetic energies are 2 eV/atoms. To minimize these effects, the kinetic energy of the cluster was decreased to 0.5 eV/atoms and the results are shown in fig.3(a)~(d). As can be seen in fig.3(d), the cluster atoms in equilibrium have well ordered structure with atomic scale nucleation, whereas it can not be seen in fig.2(d). The top and side view of equilibrium state are shown in fig.4(b). The cluster atoms are closer to each other and sit on well ordered site onto substrate while maintaining lattice distance. The defects on substrate layer are almost free and cluster atoms do not penetrate into substrate. It means that cluster atoms are epitaxally grown on the surface without damages and defects at the near interface. It is remarkably in good agreement with experiments. Moreover, the island, i.e. atomic scale nucleation sitting on substrate in fig.3(d) shows almost the same picture as the STM observation[1]. Of course, it is very difficult to directly compare experiments with simulation because different substrates were used in experiment(graphite) and calculation(Au). Actually to do simulation of the interaction Au cluster to graphite substrate like the experiment, the reliable potential is necessary to describe the interaction between graphite and Au atom, but unfortunately I can not find it yet. Therefore in this simulation, the interaction of Au cluster and Au substrate was considered because the interaction potential was relatively well described. Nevertheless, it is of interest to note that the island formed by direct deposition of clusters play an important role in epitaxial growth mechanism of ICBD. The depth distribution of cluster atoms in equilibrium for each energetic cluster energy was summarized in table 1. Here S_i is ith layer from surface and E_i is ith epilayer. Most of cluster atoms having kinetic energy of 10eV/atom are embedded in the substrate layer, with the deepest layer being the 6th one below the surface, whereas most of cluster atoms with kinetic energy less than 1 eV/atom are sit on epi-layer. The cluster atoms with kinetic energy of 0.5eV/atom are more stably distributed on the surface and formed epi-layer than any other energy. From these results, you can see that the kinetic energy of cluster atoms plays important role in obtaining good quality thin film. Figure 5 shows the kinetic energy of cluster atoms as function of time. The kinetic energy exponentially decreases after colliding until 15 pico-second and finally saturated at about 0.02eV/atom, which approximately correspond to thermal vibration energy at room temperature. It means that the cluster atoms are in almost equilibrium after 15 pico second. In conclusion, MD calculation is one of the most powerful method to understand the mechanism of ICBD. For the investigation of energy dependency of Au cluster atoms on Au substrate system, the ionized cluster atoms having 0.5eV/atom are sit on substrate without defect at the interface and form atomic scale nucleation which is in good agrement with experiment.

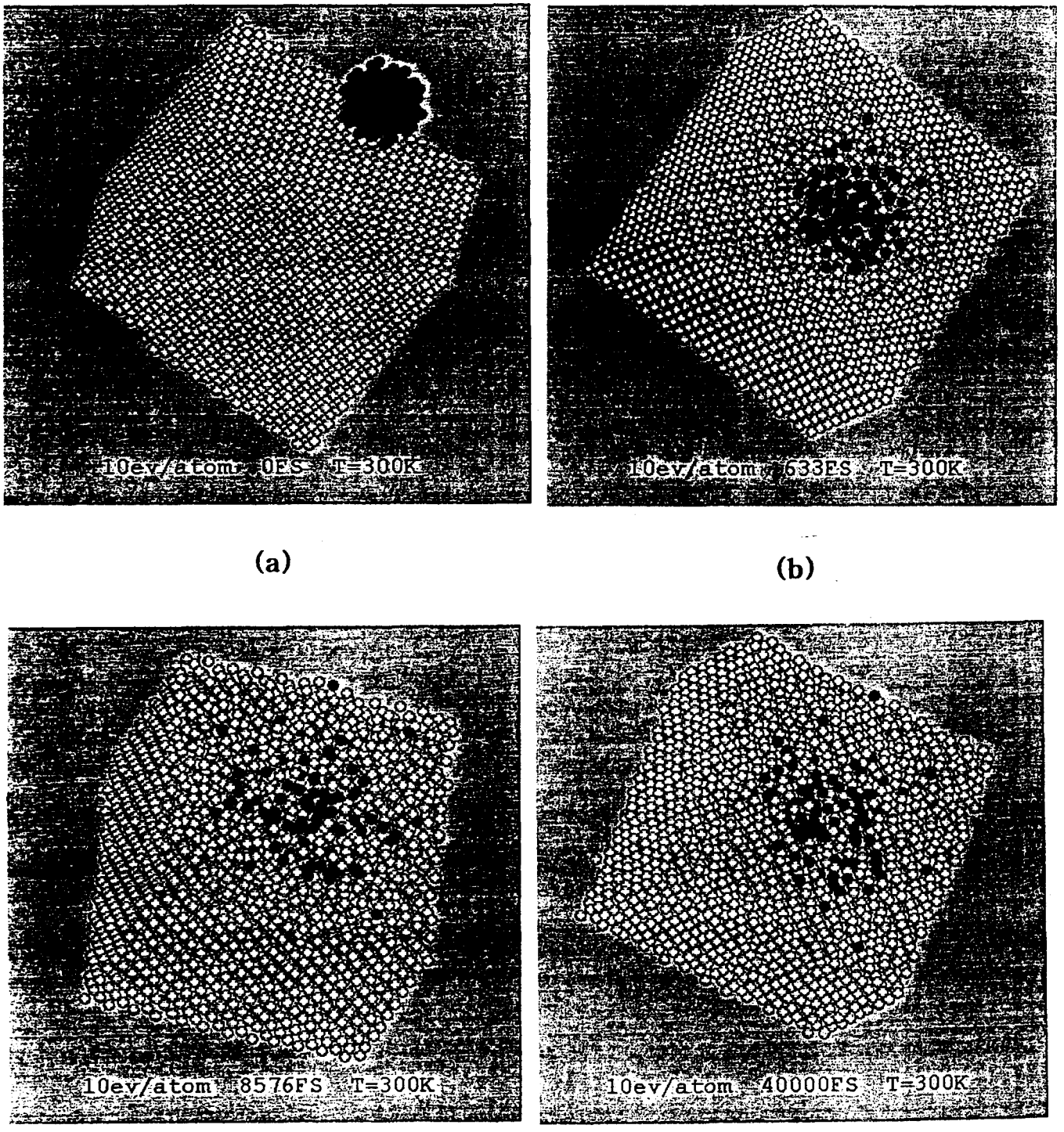


Fig. 1. Collision dynamics between Au_{95} cluster with 10 eV/atom and Au(100) substrate after 0 FS(a), 633 FS(b), 8570 FS(c), 40000 FS(d).

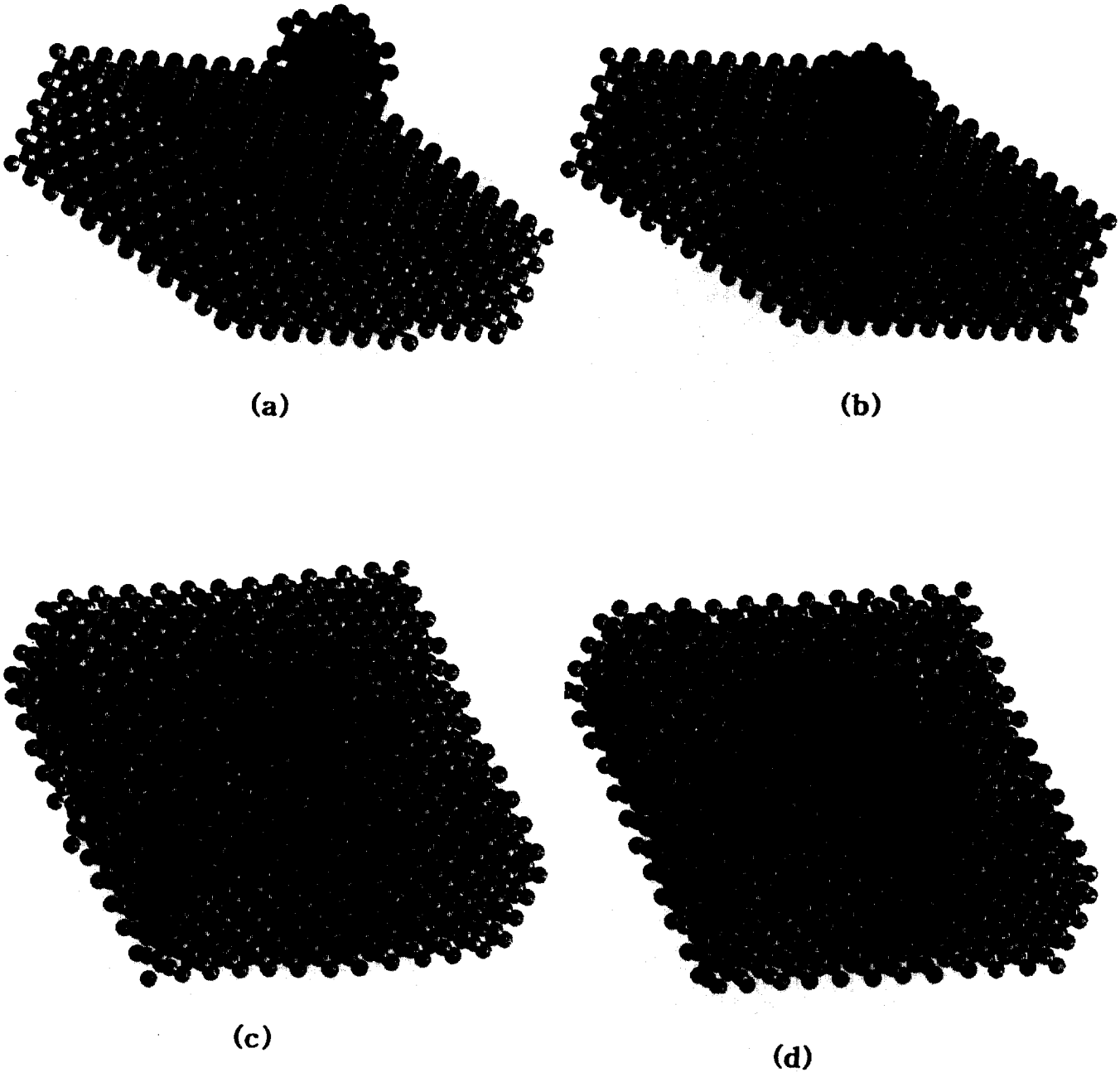


Fig. 2. Collision dynamics between Au_{55} cluster with 2 eV/atom and Au(100) substrate after 0 FS(a), 300 FS(b), 3000 FS(c), 20000 FS(d).

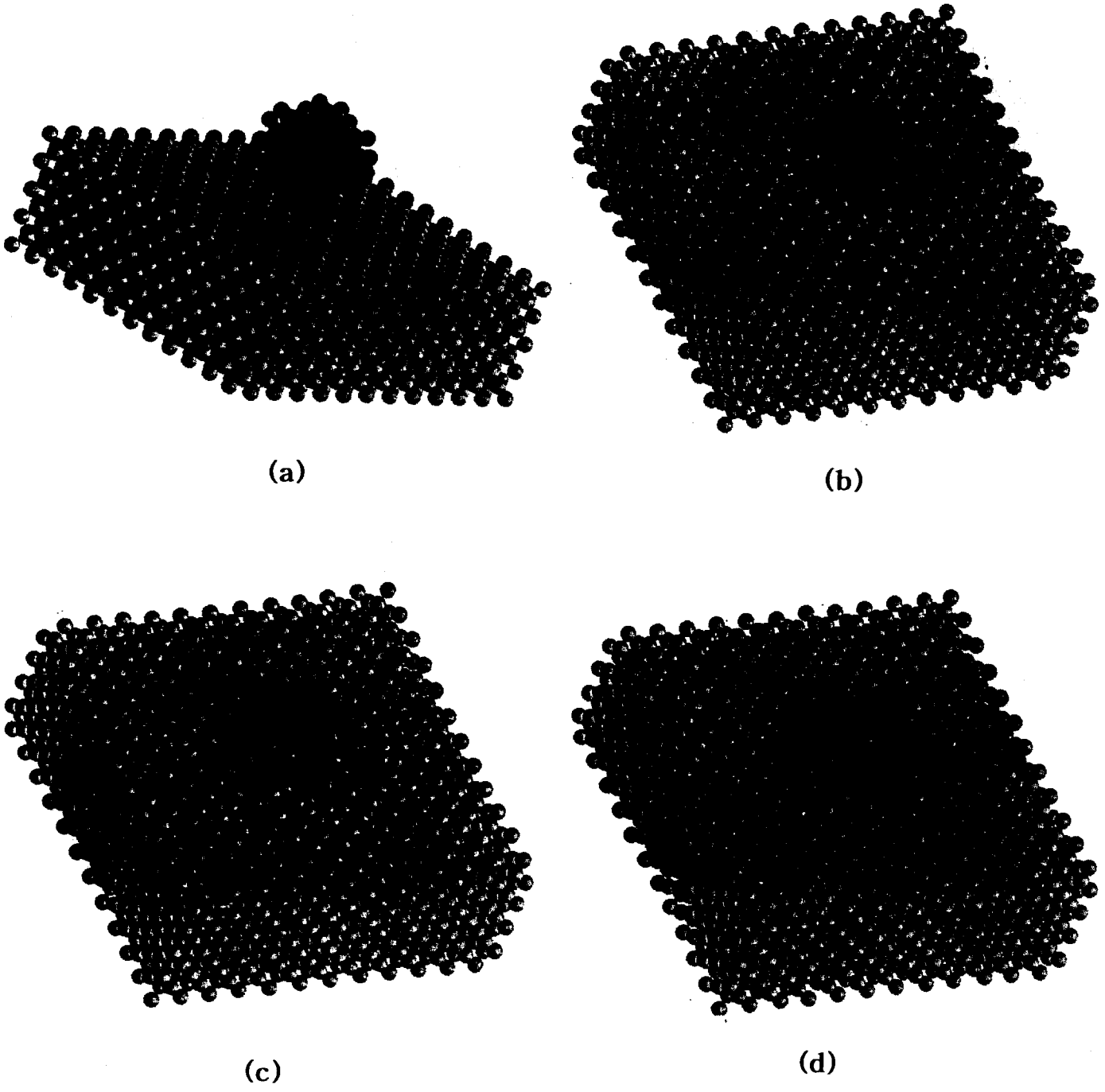
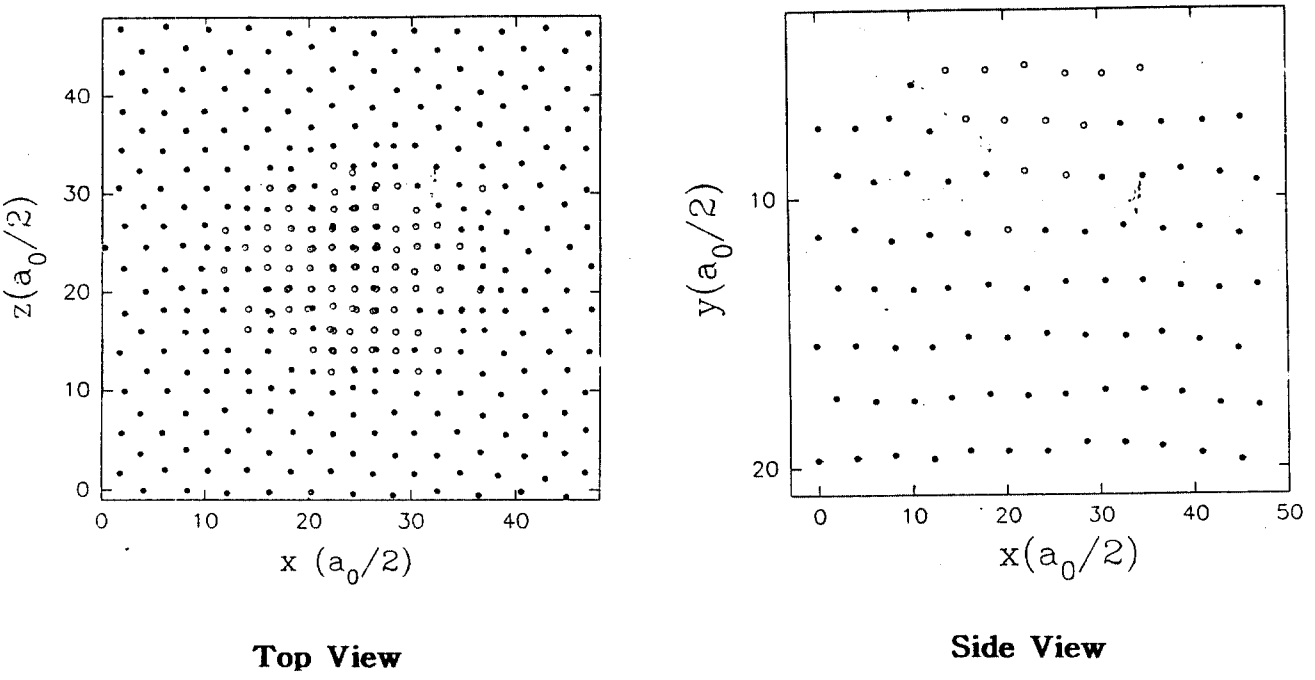


Fig. 3. Collision dynamics between Au_{95} cluster with 0.5 eV/atom and Au(100) substrate after 430 FS(a), 1200 FS(b), 2800 FS(c), 20000 FS(d).



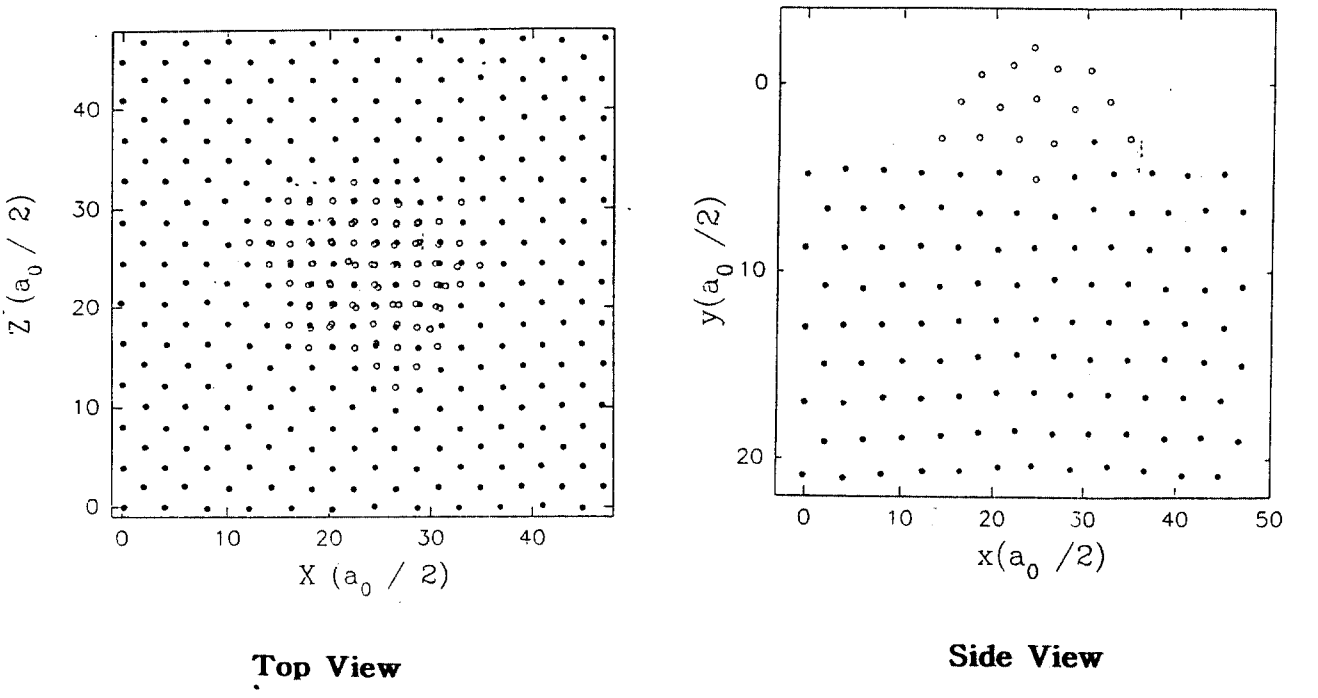


Fig. 4. The location of cluster atoms in equilibrium, Top and Side view of cluster atoms (○) on substrate atoms(●).
(a)Au_{95}(2eV/atom)→Au(100), (b)Au_{95}(0.5eV/atom)→Au(100).

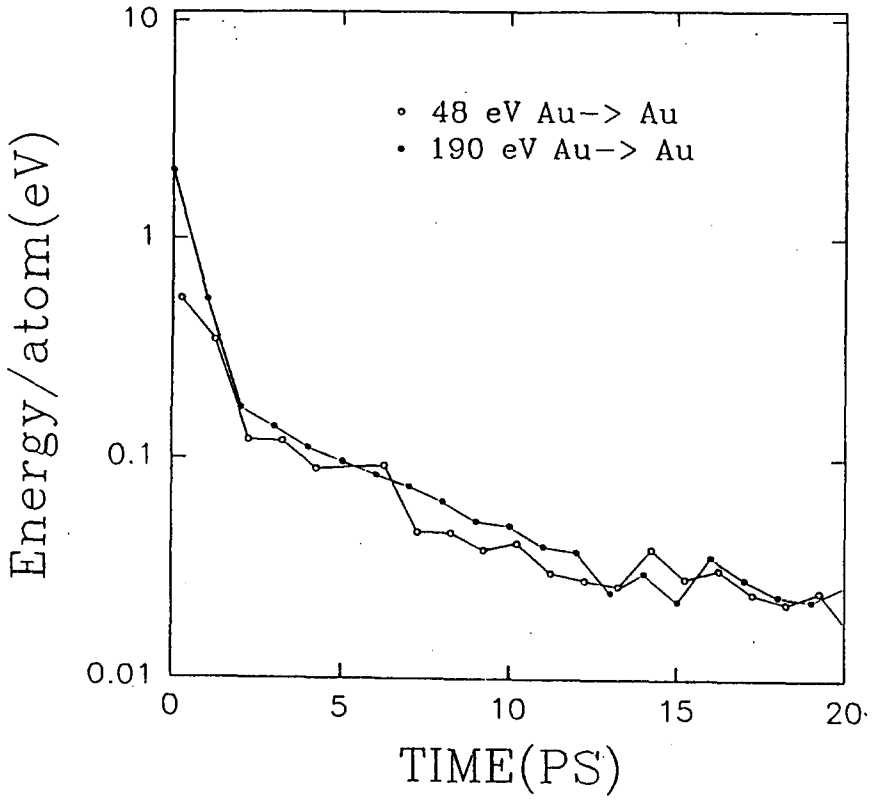


Fig. 5. Kinetic energy of cluster atoms as a function of time.

Table 1. The number of cluster atoms at every atomic layer at the end of the event.($a_0/2$: a_0 = lattice constant)

	e_5	e_4	e_3	e_2	e_1	s_1	s_2	s_3	s_4	s_5	s_6	s_7	s_8	s_9
Au_{95}(950eV)→Au 10eV/atom					11	17	20	26	13	5	3			
Au_{95}(190eV)→Au 2.0eV/atom				5	10	23	43	14						
Au_{95}(95eV)→Au 1.0eV/atom				38	39	16	2							
Au_{95}(48eV)→Au 0.5eV/atom			21	30	40	4								
Au_{95}(16eV)→Au 0.17eV/atom		14	19	27	31	4								

ACKNOWLEDGEMENTS

The authors are grateful to Prof. B. J. Garrison and Prof. N. Winograd of Pennsylvania State University for assisting us to do this work. The research was supported in part by the Korea Science and Engineering Foundation through the Science Research Center of Excellence Program(1995) and the Basic Science Research Institute Program, Ministry of Education, 1994, Project No. BSRI-94-2426. Finally, The authors are grateful to Mr. B. T. Jang, SERI, Korea for assistance of graphics.

REFERENCES

1. Isao Yamada and Gikan H. Takaoka : Jpn. J. Appl. Phys. 32 (1993) 2121.
2. I. Yamada, H. Inokawa and T. Takagi : J. Appl. Phys. 56 (1984) 2764.
3. T. Tagaki, "Ionized Cluster Beam Deposition", Noyes Pub., New Jersey, U.S.A. (1988).
4. I. Yamada, G.H. Takaoka, H. Usui, F. Satoh, Y. Itoh, K. Yamashita, S. Kitamoto, Y. Namba, Y. Hashimoto, Y. Maeyama and K. Machida : Nucl. Instrum. & Methods Phys. Res. B59/60 (1991) 216.
5. M. Adachi, S. Ikuni, K. Yamada, H. Usui and I. Yamada : Nucl. Instrum. & Methods Phys. Res. B59/60 (1991) 940.
6. B.I. Garrison and N. Winograd, Private Communication.
7. N. Winograd and B. J. Garrison, "Ion Spectroscopies for Surface Analysis",(A. W. Czanderna and David M. Hercules ed.), Plenum Press. N. Y. 1991, p45.
8. S.M. Foiles, M.I. Baskes and M.S. Daw, Phys. Rev. B33 (1986) 7893.
9. B.J. Garrison, N. Winograd, D.M. Deaven and C.T. Reimann, D.Y. Lo, T.A. Tombrello, D. E. Harrison, Jr., M.H. Shapiro, Phys. Rev B37 (1988) 7197.