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MOLECULAR DYNAMICS SIMULATION OF CLUSTER-BEAM–SURFACE IMPACT PROCESSES FOR METALLIC PHASES*

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1 Introduction

In this study we investigated the cluster–surface interactions for metallic aluminium using an optimised version of the DL_POLY molecular dynamics simulation code [1,2]. We were mainly interested in the analysis of cluster-surface impact processes, and investigated a rather large system (for both substrate and cluster). The system we considered consisted of an aluminium substrate containing 36,000 atoms and an aluminium cluster of 864 atoms. The density and temperature characteristics of the impact process were investigated in detail. It is worth noting that aluminium is widely employed in the electronics industry, for the manufacturing of thin film interconnects. Thus, studying the thin film growth processes, which involves cluster–surface impacts of aluminium and compounds, represents a challenging task of great interest. There have been a number of theoretical works in past years, which have been devoted to the cluster bombardment of metallic aluminium [3]. However, it is significant that much of the existing theoretical and computer simulation statistics available have been limited to a relatively small number of atoms in the system. On the other hand, it is well known that the processes involving the clusters and cluster-suface interactions exhibit very size-dependent dynamics (see, for example, [4]).

2 Simulation method and system

We have performed MD simulations on the Fujitsu VPP700 vector computer using the DL_POLY_2.11 code to study the cluster–surface impact process. The optimisation of DL_POLY on a vector computer, providing significant enhancements in performance, has been reported previously [2]. For the metallic system we have used the density dependent, many-body Finnis-Sinclair (FS) potential, which is available in DL_POLY in the Sutton and Chen (SC) implementation[1]. The metallic substrate was arranged in twenty layers (1800 atoms per layer) of a face-centered cubic (fcc) lattice (001) surface. The surface area was $30a_0 \times 30a_0$, with the lattice constant $a_0 = 4.0495$ Å. All the substrate atoms were considered to be dynamically mobile. Before collision the atoms in the dynamical layers were prepared at $T = 5$ K using a Berendsen thermostat. The surface was separately equilibrated at the required temperature. Slab boundary conditions in the plane (x, y) were used (there was no periodic boundary condition in $z-$direction perpendicular to the surface). The cluster was prepared in thermal equilibrium: prior to impact, with an equilibration temperature of 190 K for 20,000 molecular dynamics time steps and then cooled to $\sim$ 5 K during the next 20,000 steps (with rapid quenching every 2,000 steps) to minimize the effect of internal cluster kinetic energy on the dynamics of system. The interaction between atoms in the cluster was de-

scribed by the same potential as the substrate (i.e. the SC potential). The Al cluster was positioned at $h = 8.0 - 12.0$ Å above the center of the surface and given an incident kinetic energy towards the surface. The velocity of the center of mass of the cluster perpendicular to the surface was taken in the range $v = 0.5 - 5$ km $\cdot$ s $^{-1}$ ($E_{inc} = 0.035 - 3.5$ eV/atom). The integration time step, Δt, was taken from the interval of $1 - 10$ fs, depending on the incident energy. After separate equilibration the substrate and cluster were combined to evolve together. The simulation cell dimensions (L_x, L_y, L_z) were assigned the following values: $L_x = L_y = 30a_0$, $L_z = 20a_0$, where L_z includes the substrate–cluster separation distance. The whole system was thermalized at the required temperature for 1000 time steps before the impact .

3 Simulation results

We have considered in the present report the high energy collisions only; a more detailed analysis of the results obtained will be the subject of our following papers. The density and temperature changes of the cluster–surface system during highly energetic impacts are the least trivial and most complex events to measure. From the MD simulation data we can, however, carry out such studies with a high spatial-temporal resolution. For the purpose of analysis we have divided all the data obtained (for the particle positions, velocities, etc.) into several zones in the $z-$direction, with a_0 width each. For each zone the density and temperature changes at each time step for both substrate and cluster have been calculated. The analysis of simulation data allows one to distingush easily two major channels of the cluster–surface impact yields, viz., a soft landing and the implantation of the cluster into the substrate. An example of a cluster implantation into a solid surface is shown in Figs. 1-3, which are the results of MD simulations for a cluster incident energy of $E_{inc} = 3.5$ eV/atom ($h = 10.0$ Å) at $t = 0.5$ ps (Fig.1), $t = 3.5$ ps (Fig.2) and $t = 5.0$ ps (Fig.3), respectively: (a) top view (left); (b) side view (middle); (c) cut view (right). In the Figs. 4-6 the substrate and cluster density temperature distributions are shown. The calculated density and temperature profiles correspond to the same cluster impact energy and the same moments of time as Figs. 1-3: (a) density (left); (b) temperature (right). From the data presented by the Figs. 1-3 and Figs. 4-6 the density and energy exchange regions among the cluster and substrate can easily be understood. In an early stage of cluster impact (Fig. 1 and Fig. 4) the solid temperature in the front layers (to the cluster one) increased rapidly, though there are no visible changes for its density. Penetration of the cluster deep into the solid substrate (Fig. 2 and Fig. 5) results in a highly dynamical process: formation a new liquid-like phase during the very short time (order of several picoseconds). The temperatures of both the substrate and the cluster are very high, there is a high mixing re-

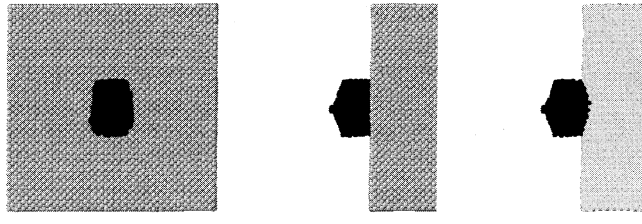

Fig. 1. The top veiw (left), side (middle) and cut (right) views of MD configurations at $t = 0.5$ ps.

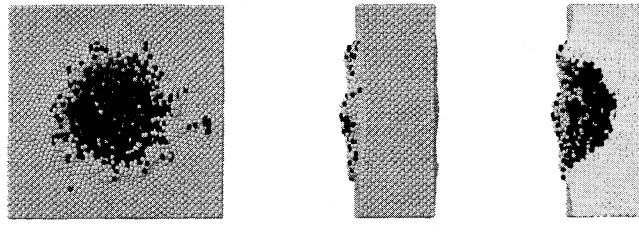

Fig. 2. The top veiw (left), side (middle) and cut (right) views of MD configurations at $t = 3.5$ ps.

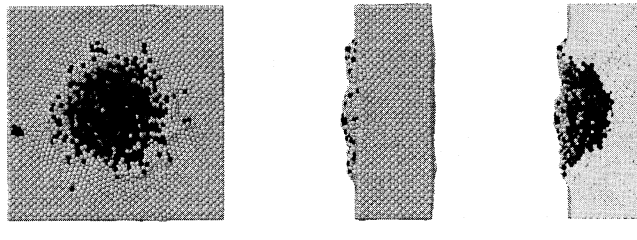

Fig. 3. The top veiw (left), side (middle) and cut (right) views of MD configurations at $t = 5.0$ ps.

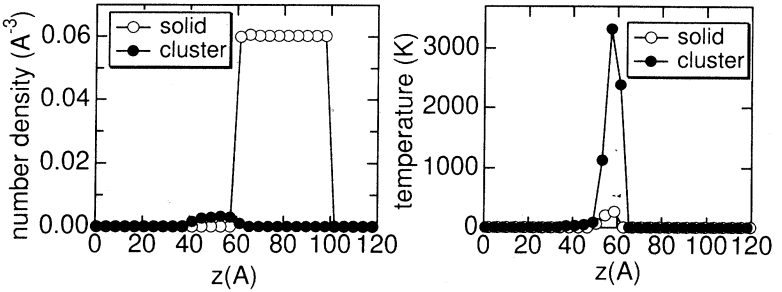

Fig. 4. The density (left) and temperature (right) profiles at $t = 0.5$ ps.

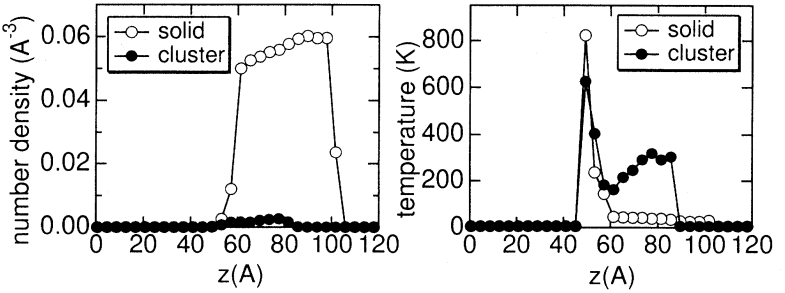

Fig. 5. The density (left) and temperature (right) profiles at $t = 3.5$ ps.

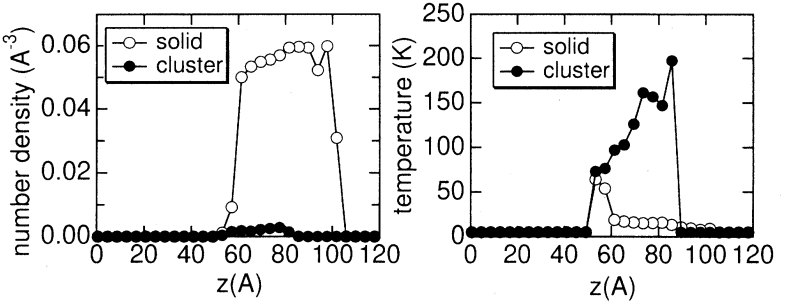

Fig. 6. The density (left) and temperature (right) profiles at $t = 5.0$ ps.

gion where the metallic phase doesn't exist any more. The cluster's temperature however is distributed over its size nonuniformly: it is high in the front and back faces, but it is lower in the central part. The density and temperature profiles of Fig. 3 and Fig. 6 show us a final simulation configuration. Although the front of the temperature wave by the cluster is still not stabilized, a thermalization condition imposed on the atoms of the substrate enabled one to control the system temperature: the substrate temperature became very close to the orginal state.

4 Conclusion

In conclusion we have used an optimised version of the DL_POLY molecular dynamics simulation code [2] to study the cluster-beam–surface impact processes for the metallic phase (aluminium). The system we have considered consisted of aluminium substrate containing 36,000 atoms and aluminium cluster of 864 atoms. The characteristics of the collision ranged from soft landing (< 0.1 eV/atom) up to higher impact energies (> 3 eV/atom). Modification of the surface, exposed to the cluster-beams, was studied by monitoring the molecular dynamics configurations of the system in real time and defining the critical impact energies, necessary to produce implantation. The density and temperature distributions in the system of cluster–substrate under highly energetic irradiations was investigated in detail.

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Холмуродов Х. и др. E11-2000-228
Моделирование процессов столкновения кластеров
с поверхностью для металлических фаз
методом молекулярной динамики

С использованием оптимизированной версии программы DL_POLY для молекулярно-динамических расчетов изучены процессы столкновения кластеров с поверхностью для металлических фаз. С помощью многочастичного потенциала Финниса–Синклэйра исследованы взаимодействия энергетических кластеров с твердой поверхностью. Характеристики столкновений изучены в широких пределах: от «мягкого» соударения (< 0,1 эВ/атом) до высоких энергий падающего на поверхность кластера (> 3 эВ/атом). Модификация поверхности под воздействием высокоэнергетических кластеров изучена на основе анализа молекулярно-динамических конфигураций в реальном времени, а также путем определения критической энергии столкновений, необходимых для имплантации кластера в материал подложки. Распределение плотностей и температур в системе кластер–подложка под действием высокоэнергетического облучения изучено детально.

Работа выполнена в Лаборатории информационных технологий ОИЯИ.

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Molecular Dynamics Simulation
of Cluster-Beam–Surface Impact Processes for Metallic Phases

An optimised version of the DL_POLY molecular dynamics simulation code has been used to study the claster-beam–surface impact processes for the metallic phase. The interaction of an energetic cluster of atoms with a solid surface was investigated using the Finnis–Sinclair many-body potential. The characteristics of the collision range from soft landing (< 0.1 eV/atom) up to higher impact energies (> 3 eV/atom). Modification of the surface, exposed to highly energetic cluster-beams, was studied by monitoring the molecular dynamics configurations of the system in real time and defining the critical impact energies, necessary to produce implantation. The density and temperature distributions in the system of cluster-substrate under highly energetic irradiations was investigated in detail.

The investigation has been performed at the Laboratory of Information Technologies, JINR.

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