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Molecular Dynamics Simulation of the interaction between cluster beams and solid surfaces

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ABSTRACT

The mechanism of the ionized cluster beam desposition has been carried out using Molecluar Dynamics Simulation. The Embedded Atom Method(EAM) potential were used in the simulation. The impact of a Au_{95}-cluster on Au(100) surface was studied for the impact energies 0.2 ~ 10eV/atom. The dependency of the impact energy of cluster beam was observed. For the cluster energy of 10eV per atom, the defects on surface were created and the cluster remained as an amorphous state on the surface. For the energy of 0.5eV per atom, the nucleation formation and defect free homoepitaxial growth were observed. But there is no dependence on the substrate temperatures between 300K and 600K with 0.5eV/atoms. For 0.5 and 2eV per atom, the cluster atoms deposited on surface became equilibrium state after 20ps. These result is in qualitative agreement with experiment. It is suggested that molecular dynamics simulation is very useful to study the mechanism of the ionized cluster beam deposition.