

나노 사이즈 Cu(111) 표면에 증착된 Pb 원자의 초기 거동에서의 비평형 핵생성에 대한 연구

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The surface uniformity of thin-film, which determines performances of the magnetic devices, is strongly affected by the shape of initial nucleus. Because of the requirement of nanosized devices, the role of nucleus is emphasized as the seed of three-dimensional growth of thin-film at the growth-restricted conditions. In the particular case of interface, Pb is a well-known surfactant material for epitaxial growth of transition metals (Fe, Co and Cu) on Cu(111) surfaces. The growth mechanism of the pre-deposited Pb monolayer (ML) on Cu(111) surface is clarified that Pb adatoms float during the epitaxial growth and form flat two-dimensional (2-D) island in non-equilibrium conditions. However, in despite of many researches of the growth mechanism were studied in Pb/Cu(111) interface, the nucleation mechanism of this system was barely known up to the present time. Moreover, the most part of the nucleation researches focused on the equilibrium condition. Therefore, through quantitative analyses, we tried to understand the atomistic nucleation mechanism of Pb/Cu(111) interface in non-equilibrium condition.

In this study, the atomic behaviors, such as surface diffusion and island formation of Pb atoms were quantitatively investigated using molecular dynamics (MD) method and density functional theory (DFT) based on ab-initio calculations, which are capable of accurate atomistic simulation of interface characteristic in multilayer thin films, to quantitatively investigate the adsorption energy of Pb/Cu(111) system. Through the atomistic behavior of Pb/Cu(111) interface, the most stable shape of nuclei was described by comparing the difference between the equilibrium and the non-equilibrium conditions.