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Inhibition of Surface Mobility of Cu Adatoms on the Cu(111) Surface via Sn Alloying[1] ZHENGZHENG CHEN, NICHOLAS KIOUSSIS, Department of Physics, California State University, Northridge, NASR GHONIEM, KING-NING TU, JENN-MING YANG, Department Mechanical and Aerospace Engineering,University of California, Los Angeles — We have investigated the effect of substitutional Sn on the diffusion of Cu-adatom on the Cu(111) surface by first principle methods. We have determined the energy landscape by accurately calculating the diffusion and adsorption energies of a Cu adatom as a function of distance from Sn. The results reveal two important electronic mechanisms: (1) each substitutional surface Sn atom introduces a forbidden adsorption region in its vicinity, within which Cu adatoms are not stable and spontaneously diffuse away from Sn; and (2) the binding of Cu adatoms close to Sn is weaker. Using the first principle calculated energy landscape, we have carried out Kinetic Monte Carlo simulations and found that Sn effectively impedes the diffusion of the Cu adatom Especially, intermetallic compound Cu_3Sn almost totally suppresses the diffusion of adatom at low and medium temperatures. Analysis of the change of surface state induced by Sn demonstrates Friedel oscillation, where the radius of the forbidden adsorption region corresponds to the first Friedel valley.

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