

Factors Affecting the Coverage Dependence of the Diffusivity of one Metal over the Surface of Another

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Various factors that can affect the coverage dependence of diffusivity in the case of surface hetero-diffusion have been analyzed. Simple Monte Carlo modeling of the diffusion process shows that diffusivity can either increase or decrease with coverage, depending on whether the interaction between diffusing atoms is repulsive or attractive. The results of more detailed simulations show that these simple predictions are reasonable. If the diffusing species undergoes first order phase transitions as a function of coverage, then important perturbations of the diffusion profiles will result. One final factor in coverage dependence of diffusivity is considered, namely the possible effects of coverage on the surface step structure. An analysis of diffusion profiles obtained for the spreading of Bi over Cu(100) shows that the major effects of coverage on diffusivity come about from the presence of phase transitions, and from the inherent coverage dependence of diffusivity in systems with short range repulsion.