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Ab-initio Study of the Erlich-Schoewebel Barriers for fcc(100)[1]
TALAT S. RAHMAN, HANDAN YILDIRIM, University of Central Florida — We present the results of density functional theory based calculations for the activation energies for the diffusion of adatoms (Cu or Ag) on Cu(100) and Ag(100) surfaces with and without steps. For Ag adatom diffusion via hopping on Cu(100), we find the energy barrier to be 0.37 eV, which is less than that (0.60 eV) of Cu adatom diffusion on Ag(100). In the presence of a step edge, we find the Erlich-Schoewebel (ES) barriers (via hopping process) for both Ag and Cu atoms on Cu(100) to be 170 meV. For Ag and Cu adatoms on Ag(100), the corresponding barriers are 50 meV and 60 meV, respectively. The ES barrier (via exchange process) for Ag on Ag(100) is found to be 20 meV and for Cu on Cu(100) it is 60 meV. The barriers for diffusion along the step edges at the lower terraces are 0.36 eV and 0.20 eV for Cu on Ag(100) and Ag on Cu(100), respectively. We trace the differences in the diffusion barriers of the homo-and hetero-epitaxial systems to the differences in the corrugation of the potential energy surface, and discuss the implications for homo-and heteroepitaxial growth on these surfaces.

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