Cu/Ag EAM potential optimized for heteroepitaxial diffusion from ab initio data

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Low temperature in situ STM studies of Cu islands on Ag(111) by Weaver at UIUC observed anomalously fast diffusion for a subset of small islands. To study the dynamics of Cu island diffusion at 130K and below, we use ultrasoft pseudo-potential GGA calculations to optimize an embedded atom method (EAM) potential. The relative energies of different Cu monomer and dimer states as well as the relaxed geometries comprise the ab initio data set. We modify the Mishin Cu-Ag EAM potential[1]—specifically the Cu-Ag and Cu-Cu pair interactions—and apply the new potential to test the diffusion dynamics of Cu monomers, dimers, and trimers on Ag(111). The diffusion barriers calculated for the monomer and dimer systems compare well to experimental values.[2] Initial results for larger islands confirm the effect of lattice mismatch on cluster diffusion. This work is supported by NSF/DMR grant 0703995.

[1] P. L. Williams et. al., Modelling Simul. Mater. Sci. Eng. **14**, 817 (2006).

[2] K. Morgenstern et. al., Phys. Rev. Lett. **93**, 056102 (2004).