

Abstract Submitted
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Heterogeneity in ultrathin films simulated by Monte Carlo method¹ JIEBING SUN, Department of Physics, University of New Hampshire, JAMES B. HANNON, IBM T. J. Watson Research Center, GARY L. KELLOGG, Sandia National Laboratories, Albuquerque, NM, KARSTEN POHL, Department of Physics, University of New Hampshire — The 3D composition profile of ultra-thin Pd films on Cu(001) has been experimentally determined using low energy electron microscopy (LEEM).^[1] Quantitative measurements of the alloy concentration profile near steps show that the Pd distribution in the 3rd layer is heterogeneous due to step overgrowth during Pd deposition. Interestingly, the Pd distribution in the 2nd layer is also heterogeneous, and appears to be correlated with the distribution in the 1st layer. We describe Monte Carlo simulations that show that correlation is due to Cu-Pd attraction, and that the 2nd layer Pd is, in fact, laterally equilibrated. By comparing measured and simulated concentration profiles, we can estimate this attraction within a simple bond counting model. [1] J. B. Hannon, J. Sun, K. Pohl, G. L. Kellogg, *Phys. Rev. Lett.* **96**, 246103 (2006)

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