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**Local surface structure and composition determination  
by low-energy electron microscopy and Monte Carlo simulation**

JIEBING SUN, Univ. of New Hampshire, JAMES B. HANNON, IBM Research Center, GARY L. KELLOGG, Sandia National Labs, KARSTEN POHL, Univ. of New Hampshire — It has been long pursued to accurately measure surface structure and composition with high temporal and spatial resolutions. Modern surface analytical techniques, however, either have to assume a homogeneous surface structure, or have only a very limited sensitivity to subsurface or chemical composition. We have developed a novel analysis technique to overcome these limitations [1-2]. We are able for the first time to measure a complete 3D composition map of the first three surface layers in real time by analyzing low-energy electron microscopy imaging intensity dynamically. We have demonstrated that a lateral spatial resolution of about 8.5 nm can be achieved to unravel the origin of the heterogeneous PdCu surface alloy grown on a Cu(001) substrate. A fundamental step-overgrowth mechanism has been identified to be responsible for the heterogeneity developing around steps, a generic mechanism relevant to many thin-film systems. Furthermore, Monte Carlo simulations indicate that the favorable NN Pd-Cu bonding is responsible for the heterogeneity in the PdCu system and not a slow diffusion process. [1] J. B. Hannon *et al.*, Phys. Rev. Lett. 96, 246103(2006) [2] J. Sun *et al.*, Phys. Rev. B (scheduled for publication 15 Oct 2007)

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