

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Effect of misfit dislocation on surface diffusion¹ MARAL AMIN-POUR, University of Central Florida, OLEG TRUSHIN, Yaroslavl Branch of the Institute of Physics and Technology of Russian Academy of Sciences, Yaroslavl, Russia, TALAT RAHMAN, University of Central Florida — We apply molecular dynamics and molecular static methods to study the effect of misfit dislocations on adatom diffusion in close proximity to the dislocation core in heteroepitaxial systems, using many body interaction potentials. Our system consists of several layers (3-7) of Cu placed on top of a Ni(111) substrate. The misfit dislocation are created with the core located at the interface between the Cu film and Ni substrate, using a method described earlier[1]. Presence of the defect inside the structure leads to formation of strain fields on the surface, which affects adatom diffusion. To make quantitative estimates of the effect, we compare adatom diffusion on surfaces with misfit dislocation underneath, and on those without such defects. We find that presence of the defect under the surface strongly affects the adatom trajectory, creating anisotropy in atomic diffusion, even for the 7 layer Cu film. We also calculate the potential surface energy available to the adatom and compare the energy barriers for adatom diffusion in the core region and on the defect free sample. ref1. O Trushin *et al*, J. Phys.: Condens. Matter 21 084211 2009

¹Work supported in part by NSF grant ITR-0840389

Maral Aminpour
University of Central Florida

Date submitted: 20 Nov 2009

Electronic form version 1.4