Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Effect of tensile misfit dislocation on diffusion of Ni adatom on Ni/Cu(111): a Molecular Dynamics study[1] OLEG TRUSHIN, Yaroslavl Branch of the Institute of Physics and Technology of RAS, Yaroslav, Russia, MARAL AMINPOUR, TALAT S. RAHMAN, Physics Department, University of Central Florida — We apply molecular dynamics and molecular static methods to calculate the effect of tensile misfit dislocation on Ni adatom diffusion for Ni/Cu(111) system and compare the results with those calculated previously for Cu adatom on the Cu/Ni(111) system [1] which has compressive dislocation. Our Ni/Cu(111) substrate model system consists of 5 layers of Ni on top of a 7-layer Cu(111) slab which after energy minimization displays an isolated misfit dislocation buried at the Cu-Ni interface, causing the Ni film to be under tensile stress. In contrast to the isotropic trajectory that emerges on a defect-free surface, in this tensile stressed system we find that presence of the defect under the surface strongly affects the adatom trajectory, introducing anisotropy in atomic diffusion similar to compressive system, but with the difference: tensile misfit dislocation enhances diffusion in the direction perpendicular to the misfit dislocation line and decreases it in the direction parallel to it, whereas compressive dislocation induces the opposite behavior. We present the calculated energy barriers for the adatom and compare them with adatom diffusion on defect – free and on the surface containing compressive dislocation.

[1] M. Aminpour, O. Trushin, and T. S. Rahman, Physical Review B, 84, 035455 (2011).

[1]The work was supported in part by DOE grant No. FG0203ER46354.

Volodymyr Turkowski
Physics Department, University of Central Florida

Date submitted: 22 Nov 2011 Electronic form version 1.4