Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Semi-coherent Fe(001)/MX(001) interfaces DAN FORS, GÖRAN WAHNSTRÖM, Chalmers University of Technology — Using ab initio calculations we investigate interface energies and structures for the semi-coherent Fe(001)/MX(001) interface systems. We apply a continuum approach using the Peierls-Nabarro model in order to account for the elastic displacements arising from the lattice misfit and the periodic misfit dislocations in the interface. The chemical part of the interface energy is obtained by using density functional theory calculations. We find that the Fe/MN systems show decreasing trends along the 3d, 4d and 5d element rows corresponding to stronger bonding to Fe. In contrast the Fe/MC systems show a maximum for the Ti group. The trends and differences have been explored using projected density of states and charge density analysis. The results show a stong covalent bonding between Fe and C(N) when the two atoms are aligned on top of each other, but the hybridization itself can't account for the differences along the rows. Instead the trend appears to be due to the metallic interaction between the Fe atom and M atom in the interface layer. We also find that the Fe/MX-interfaces have large misfits, which causes that many atoms will be unfavorable positioned and the elastic energy will constitute a significant part of the interface energy.

Dan Fors
Chalmers University of Technology

Date submitted: 19 Nov 2007 Electronic form version 1.4