Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Mg(0001): Electronic structure features controlling the limit of and reactivity in the thin-film regime, stacking fault of Mg adislands and adatom self-diffusion[1] MARISOL ALCANTARA ORTIGOZA, MARAL AMINPOUR, TALAT S. RAHMAN, University of Central Florida — We analyze the electronic structure of the Mg(0001) surface as a function of slab thickness to reveal the features that control chemical reactivity of films of less than 17 layers. The thickness dependence of the oxidation rate of Mg thin films is directly related to the in-plane-PLDOS(E) of the first- and second-layer atoms around the Fermi level. Regarding the origin of the stacking fault - which is attached to a Friedel-oscillation-driven charge density pocket at the fcc site, we find that the role of the charge-density pocket is that of strengthening the substrate bonds since adsorption at the fcc site charge is distributed among surface atoms enhancing their mutual binding. Charge-density analyses, however, are only indirect evidence that the stacking fault is caused by Mg Friedel oscillations. To strengthen our arguments, we thus test an additional material: Be(0001) – another hcp sp- and nearly-free-electron metal that is also strongly influenced by Friedel oscillations. Comparison of Mg(0001) and Be(0001) shows that the charge density enhancement at the fcc site for Be(0001) is dramatically larger than that found for Mg(0001). Most importantly, Be(0001) provides more evidence that the stacking fault preference is driven by the Friedel oscillations. Namely, the Be monomer on Be(0001) not only also prefers the fcc stacking fault site than the hcp one but the stacking fault energy is strikingly large: 44 meV.

[1]This work was supported in part by DOE grant DE-FG02-07ER46354.

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Date submitted: 15 Nov 2013 Electronic form version 1.4