Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Structure, bonding, and adhesion of $MoSi_2$/Fe and SiO_2/$MoSi_2$ from first principles DE-EN JIANG, UCLA, EMILY CARTER, Princeton University — The high-melting-point compound $MoSi_2$ is a promising candidate for a high temperature coating on iron steels and refractory metals. A coherent silica scale that forms leads to the high temperature oxidation and corrosion resistance of $MoSi_2$. Using periodic density functional theory techniques we examine the adhesion strength, interfacial geometry, and bonding characteristics of $MoSi_2$/Fe and SiO_2/$MoSi_2$ interfaces. We predict that $MoSi_2$/Fe interfaces have intrinsic adhesion energies of $\sim$3.85 J/m^2, significantly stronger than the adhesion between iron and other ceramic coating materials such as ZrC and TiC. We find that the bonding at the interface is local, with covalent character exhibited between Fe-Si and Fe-Mo across the interfaces. Experiment shows that amorphous (a) silica forms on $MoSi_2$. We use β-cristobalite to model a-silica, since they have similar local structure. We find that Si-O covalent bonding dominates the interfacial adhesion of SiO_2/$MoSi_2$, yielding strong adhesion energy of 5.75 J/m^2. These very high interfacial adhesion energies suggest that $MoSi_2$ indeed should be a quite thermally stable coating for steels.

De-en Jiang
UCLA

Date submitted: 24 Nov 2004 Electronic form version 1.4