Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

The effect of Fe atoms on the adsorption of a W atom on W surfaces JEFFERY HOUZE, SUNGHO KIM, SEONG-JIN PARK, RANDALL GERMAN, MARK HORSTEMEYER, SEONG-GON KIM, Mississippi State University — We report ab-initio calculations on the effect of iron (Fe) atoms on the adsorption of a tungsten (W) atom on W(100), W(110), and W(111) surfaces. The adsorption of a W atom on the clean W surfaces is compared with the adsorption of a W atom on a monolayer of Fe atoms covering the W surfaces. The total energy of the system is computed as the function of the height of the W adatom. For the W(100) surface I will show that the W atom first adsorbs onto the Fe monolayer. Then the W atom can replace one of the Fe atoms through a path with a moderate energy barrier and reduce its energy further. This intermediate site makes the adsorption (and desorption) of W atoms a two-step process in the presence of Fe atoms and lowers the overall adsorption energy by nearly 2.4 eV. Similar processes for adsorption will be presented for the (110) and (111) surfaces. Our result provides a fundamental mechanism that can explain the activated sintering of tungsten by Fe atoms.

Jeffery Houze
Mississippi State University

Date submitted: 27 Nov 2007 Electronic form version 1.4