

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Calculated atomic arrangement and impurity bonding at a κ -Alumina – Al(771) interface.¹ PETER J. FEIBELMAN, Sandia National Laboratories — First principles optimization of a κ -Alumina – Al(771) superlattice shows that the incompressible oxide causes substantial disorder in the adjacent, soft metal layers. An H “probe atom” is found to bind best in the disrupted metal region, suggesting that this is the locus of initial failure of a protective oxide layer.

¹Work supported by the DOE Office of Basic Energy Sciences, Division of Materials Science and Engineering. Sandia is operated by the Lockheed Martin Co. for the U.S. DOE’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Date submitted: 12 Nov 2007

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