

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Liquid-metal embrittlement in Iron: surface energy reduction of Fe(110) upon Hg, Pb and Bi adsorption¹ LIN-LIN WANG, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, THIERRY AUGER, Ecole Centrale Paris MSSMAT, UMR CNRS 8579, DUANE D. JOHNSON, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign — Recent crack propagation measurements in the presence of Hg, Pb, and Bi liquid overlayers have shown that Hg is the strongest embrittler. These observations are in distinct contrast to previous theoretical predictions for submonolayer coverage, where Hg decreases the Fe(110) surface energy the least amongst the three liquid metals. Using density functional theory with molecular dynamics, we quantitatively reproduce the experimental observation, and show that there is a crossover in the reduction of surface energy depending on coverage. We analyze the electronic structure effects responsible for the reversal trend in the surface energy reduction. The Hg-Fe interaction involves significant hybridization between Hg 5d bands and Fe 3d bands for liquid-like overlayer, while, for Pb and Bi, the interaction with Fe is best described via polarization, which diminishes in strength with more than one monolayer coverage.

¹DOE/Catalysis DE-FG02-03ER15476 and DOE/BES DEFG02-03ER46026.

Lin-Lin Wang
Department of Materials Science and Engineering,
University of Illinois at Urbana-Champaign

Date submitted: 01 Dec 2009

Electronic form version 1.4