

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

First Principles Study of Bismuth Films at Transition Metal Grain Boundaries¹ QIN GAO, MICHAEL WIDOM, Carnegie Mellon University — Recent experiments suggest that Bi impurities segregate to form bilayer films on Ni and Cu grain boundaries but do not segregate in Fe. To explain these phenomena, we study the total energies of Bi films on transition metal (TM) $\Sigma 3(111)$ and $\Sigma 5(012)$ grain boundaries (GBs) using density functional theory. Our results agree with the observed stabilities. We propose a model to predict Bi bilayer stability at Ni GBs which suggests that Bi bilayer is not thermodynamically stable on low energy (111) twist CSL GBs but is stable in most (100) twist CSL GBs. We investigated the interaction and bonding character between Bi and TMs to explain the differences among TMs based on localization of orbitals and magnetism.

¹Financial support from the ONR-MURI under the grant NO. N00014-11-1-0678 is gratefully acknowledged.

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Date submitted: 15 Nov 2013

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