Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Tight-binding calculations of the band structure and phases of Zinc and Cadmium CHRISTOPHER ASHMAN, DIMITRIS PAPACONSTANTOPOULOS, MICHAEL MEHL, Naval Research Laboratory — Tight-binding calculations for Zn and Cd in a variety of crystal structures have been examined using the NRL non-orthogonal tight-binding model with parameters selected to accurately fit the first-principles results. These parameters correctly predict hcp to be the stable crystal structure for both Zn and Cd and reproduce well the first-principles band structure. We have calculated other properties, which were not included in the fit, such as elastic constants, bulk phases, the vacancy formation energy and phonon frequencies. We find good agreement with available calculations and experiment.

Christopher Ashman
Materials Science and Technology Division, Code 6390
Naval Research Laboratory

Date submitted: 06 Dec 2004 Electronic form version 1.4