Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Thermodynamic model for the structure of the 90 degree partial dislocation in diamond cubic semiconductors.[1] S. P. BECKMAN, The University of Texas at Austin, D. C. CHRZAN, The University of California at Berkeley — Recent studies of the 90 degree partial dislocation in diamond cubic semiconductors indicate that the structure of the core is not homogeneous, but rather is a combination of reconstructions and low energy structural excitations, such as kinks and anti-phase defects. As a result, direct investigation of the macroscopic properties of dislocation core by *ab initio* methods is unfeasible. A model is presented that maps the complicated structure of a dislocation core onto a one-dimensional spin lattice. At each lattice site two spins are present, one to represent the reconstructed bonds, and the other kink structures. The model is sufficiently complex to allow expression of the essential nature of the structural excitations along a dislocation line. This Ising-like model can be investigated within a Monte Carlo framework.

[1]This work is supported by the Department of Energy, Office of Science, Basic Energy Sciences. Computational resources were provided by NERSC.

S. P. Beckman
The University of Texas at Austin

Date submitted: 30 Nov 2005 Electronic form version 1.4