Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Tight binding models derived from k-dot-p theory C. E. PRYOR, Dept. of Physics and Astronomy, University of Iowa, M.-E. PISTOL, Dept. of Physics, Lund University, Sweden — Calculations of the electronic properties of semiconductor nanostructures rely on one of three different methods: tight-binding, pseudopotentials, or k-dot-p theory. The first two are well suited to modeling small scale structures, however their parameters must be fitted to bulk properties, which can be a complicated procedure, especially for tight-binding. In contrast, k-dot-p theory is best at describing large nanostructures in which the placement of individual atoms is not important, and the parameters of k-dot-p theory are directly related to experimentally determined quantities. To bridge the gap between atomistic and large scale models, we will present a method for constructing tight-binding models directly from k-dot-p theory by considering a real-space representation of k-dot-p theory with finite differences on a grid which matches the desired crystal lattice. Conversely, given a tight-binding model it is also possible to construct an equivalent k-dot-p theory in the long wavelength limit

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Date submitted: 30 Nov 2005 Electronic form version 1.4