Homework Assignment on the Electronic Structure

Dragica Vasileska and Gerhard Klimeck
(ASU, Purdue)

It is well known that free electrons exhibit the free electron mass m_0 and that electrons in a crystal with periodic potential are described with effective mass m_{eff} that is derived from the dispersion relation. In other words the curvature of the bands is inversely proportional to the effective mass of the carriers moving in that potential. It is also well known that periodicity of the potential opens gaps in the dispersion relation at the Brillouin zone edges. Using the Periodic potential tool installed on the nanoHUB plot the dispersion relation for square wells in the reduced zone description and for Coulomb potentials in the expanded zone description. For the square potential well use (a) W=8 A, a=1 A, (b) W=7.5 A and a=0.5 A, (c) W=7.1 A and a=0.1 A. For the Coulomb potential use: (a) W=8 A, a=2 A, (b) W=8 A, a=3 A, (c) W=8 A, a=4 A. Comment on:

(a) The variation of the curvature of the bands with decreasing the width of the barrier.
(b) The variations of the band-gaps with the width of the wells that determines the cross-talk between neighboring wells.
(c) The variation in the dispersion relation for square vs. Coulomb potential.
(d) Discuss the free-electron limit for the both types of wells.