1.0 Introduction

Before the one-dimensional Schrödinger equation can be solved in order to find the bound electron states in a QCL's quantum well landscape, the potential energy profile of the QCL must be known. The potential energy $V(z)$ is the sum of the conduction-band edge E_c, the externally applied bias voltage eV_{app}, and the built-in potential $e\Phi$ due to space charge. The conduction-band edge is a series of quantum wells because the differing layers of semiconductor material have different band-gaps and band alignments. The built-in potential is found by solving the Poisson equation when the space charge is known. The bias voltage can be thought of being as contained in the built-in potential, because it is a constant, linear function which can be accounted for by applying the proper boundary conditions to the Poisson equation. With this in mind, the total potential energy becomes:

$$V(z) = E_c(z) - e\,\Phi(z)$$

Here e is the electron charge, needed to convert the electrostatic potential to a potential energy.

2.0 The Conduction-band Edge

Because the Poisson equation takes care of space charge effects arising from the heterojunction of thin semiconductor layers, the conduction band-edge can be assumed to be the same as that for a large bulk piece of material. The location of the conduction band edge is calculated as the sum of the valence-band edge $E_{v,abs}$ on an absolute scale plus the energy band gap E_g:

$$E_c = E_{v,abs} + E_g$$

The valence-band edge energies on an absolute scale are taken from the Van de Walle[1] values, and are calculated as a function of alloy concentration according to a linear model:

$$E_{v,abs} = E_{v,0} + E_{v,1}\,x$$

Here x is the alloy concentration, $E_{v,0}$ is the Van de Walle absolute-scale valence band edge of the pure material (e.g. GaAs), and $(E_{v,0} + E_{v,1})$ is the Van de Walle absolute-scale valence band edge of the fully alloy material (e.g. AlAs).

The energy gap is temperature and alloy dependent and so the Varshni[2] empirical form is used to calculate it:

$$E_g = (E_0 + E_1 x + E_2 x^2) - \frac{(\alpha_0 + \alpha_1 x) T^2}{T + (\beta_0 + \beta_1 x)}$$

Here, T is the lattice temperature; x is the alloy concentration; E_0, E_1, and E_2 are the zero-temperature band gap parameters; and α and β are the Varshni form parameters. All of these parameters are different for each material and can be found in the literature. For ease of use, the code presents the most common QCL semiconductor materials to the user as layer material options, and their corresponding material parameters are automatically loaded by the code from a material parameters file.

[1] C. G. Van de Walle, "Band lineups and deformation potentials in the model-solid theory." Phys. Rev. B, 39:3 (1989).

[2] I. Vurgaftman, J. R. Meyer, L. R. Ram-Mohan, "Band parameters for III-V compound semiconductors and their alloys." J. Apply. Phys. 89:11 (2001).