1.0 Introduction

A quantum cascade laser typically consists of a stack of nanoscale epitaxial semiconductor planar layers. The material is uniform and near-infinite in the directions transverse to crystal growth (the x-y dimensions). As a result, all of the properties in a QCL depend only on the growth direction (the z dimension). Because the material changes in the growth direction, all material properties, such as the dielectric constant and effective mass, are functions of z and cannot be treated as constant. The conduction band edge, the potential that electrons experience via the Schrödinger equation, the electron wavefunctions, and the space charge are all functions of z. In order to solve the physical equations numerically, we must represent every function of z as a set of values over a discrete grid of z location points. Practicality, efficiency, and accuracy dictate that all properties that are functions of z should be defined across the same grid of points. The code therefore establishes a location grid data structure before solving any physical equations. The location of all z points is held fixed through-out the entire QCL computation and all variables are calculated at these z points.

2.0 Create Location Grid

Our code models three repeated periods of the core QCL structure. While a typical QCL has over 70 periods, three periods is sufficient for computations if we enforce periodic boundary conditions. (The potential is not strictly periodic because there is a net potential drop across one period due to the applied bias. More accurately, all of the variables are periodic after the bias has been divided out.) One might think that one period is sufficient if periodic boundary conditions are enforced. It turns out that many electron wavefunctions are longer than one period, so that more than one period is needed to get their full extent. In order to enforce periodicity and avoid edge effects, all variables are solved across all three periods, and then the more accurate values in the central period are copied to the outer periods.

The location grid starts at $z = 0$, marking the point where electrons begin cascading down the structure, and extends to $z = 3L$, where L is the length of one period. The positive z direction is the direction of the electrons' net motion as they cascade down through the structure.

One option for choosing location grid points is to simply distribute them uniformly between the endpoints according to some density the user specifies. This option would allow standard integration techniques such as Simpson's rule to be used, as well as simplify the numerical representation of differential equations. This option, however, leads to poor accuracy. The reason for accuracy degradation is that the material layer widths in a QCL are highly non-uniform, and the wavefunctions depend strongly on the layer widths. Using a uniform grid of z points would require rounding layer interface locations to the nearest grid point, significantly altering their widths, and therefore degrading

all subsequent calculations.

A second option is used by our code. Grid points are set exactly at the location of every material layer interface. Grid points are then spread uniformly within each layer according to a density specified by the user. By using this approach, the grid is very close to uniform, but still preserves the exact layer widths. Because the grid is non-uniform, the non-uniform trapezoidal method must be used to perform numerical integrations over z instead of Simpson's rule. Also, when expanding differential equations, the step size h of the derivative depends on the location and is not a constant.

3.0 Populate Grid with Material Properties

All of the position-dependent properties that stay constant are calculated at the beginning. These properties are essentially material properties that are assumed to behave as in bulk. The band-gap, band alignment, and the donor ionization density are discussed elsewhere. All other material properties are calculated at each grid point using a linear model such as:

$$m = m_0 + m_1 x$$

Here x is the alloy concentration at the grid point, m_0 is the property value when there is no alloy present, and m_1 is the property value change that occurs at a full alloy concentration.