A New Solution Method for Mixed Boundary Value Problems: Applications to Current Injection in Semiconductor Lasers

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BIOGRAPHY

Gregory C. Dente: Gregory C. Dente received the Ph. D. degree in physics from Washington University, St. Louis, MO in 1975. In 1979 he joined the Perkin-Elmer Corporation, Danbury, CT. Five years later he moved to Albuquerque, where he began his own consulting business in 1985. Since completing his doctoral research in the area of quantum electrodynamics, his research experience has covered physical optics phenomena, laser theory, resonator and optical design and optical metrology. His current research efforts are in the areas of semiconductor lasers and optics.



TECHNICAL ABSTRACT

We have developed an iterative procedure for calculating solutions to *Mixed Boundary Value Problems*. The method has proven to be practical and accurate. First, we demonstrate the method by calculating injection current profiles from a metal contact plane into a single layer of finite conductivity material. Next, we show how the method readily adapts to much more complicated cases, such as injection current profiles for Quantum Cascade Laser (QCL) geometries.

There are many solution methods for boundary value problems specified by either *Dirichlet* or *Neumann* boundary conditions. In the Dirichlet case, the solution is specified on the boundary while in the Neumann case the normal derivative is specified. A third class of boundary conditions, the *Mixed* boundary conditions, receives far less discussion. In this case, the solution is specified over part of the boundary, while the normal derivative of the solution is specified over the remaining part. Indeed, methods for solving the mixed case are still very limited and usually applicable to a very few specialized geometries. Unfortunately for semiconductor device researchers, the problem of current injection into epitaxial structures falls into this nearly intractable category of mixed boundary value problems.

Consider a metal stripe contact formed by etching through an insulating layer. The contact is maintained at a constant voltage on the top surface, while the lowest surface is totally metallized and maintained at zero potential. Assuming nonisotropic conductivities and no charge accumulation, the electrostatic potential in each epitaxial layer, l, is given by a solution to the following equations subject to mixed boundary conditions at the contact layer y = L:

$$\frac{\partial^2 V}{\partial x^2} + \left(\frac{\sigma_y}{\sigma_x}\right)_l \frac{\partial^2 V}{\partial y^2} = 0 \qquad (l = 1, 2, 3, ...)$$

 $V(x, y = L) = V_{app}$ "voltage fixed for x on contact" $\frac{\partial V}{\partial y}(x, y = L) = 0$ "no y - current for x off contact" V(x, y = 0) = 0 "zero potential"

Additionally, voltage and current continuity are enforced at each interface. Although there are several difficult aspects to the injection process, the mixed boundary conditions at y=L prove to be the most challenging. Often, injection

current calculations replace the constant contact voltage with a constant current assumption. This changes the mixed boundary conditions to artificial Neumann conditions. All contact current crowding features are, thereby, totally lost. This approach is taken in Reference 1.

Our iterative method, on the other hand, relies on connection formulas that exist between the voltage, *V*, and the normal derivative of the voltage on the boundary of the problem domain. For current injection, these are given as

$$\frac{\partial V(x)}{\partial y} = \int dx' H(x - x') V(x')$$
$$V(x) = \int dx' K(x - x') \frac{\partial V(x')}{\partial y}$$

in which the kernel K is the inverse of the kernel H. We begin to iterate on these connection formulas by first guessing a potential V(x) that is equal to the specified voltage on the contact. We then calculate an estimate to the normal derivative using the kernel H and correct this estimate to the specified Neumann conditions off the contact. This interim value of the normal derivative is then used with the kernel K to generate a better prediction for V off the contact. The cycle is then repeated. For the problems that we present, the iterative convolution calculations are easily done in Fourier transform space using numerical Fast-Fourier-Transform (*FFT*) methods, as well as easily derived analytical expressions for the transforms of the kernels. In most cases, the method converges quickly and accurately. This new iterative method allows for modeling of lateral current spreading and current crowding at the edges of a contact, as well as self-consistent current redistribution in the laser active region. A typical calculated current injection profile on the contact plane, demonstrating the pronounced current crowding at the contact edges, is shown in Fig. (1).



Figure 1. Calculated current injection profile on the contact plane.

1.) Becker C., Sirtori C., "Lateral Current Spreading in Unipolar Semiconductor Lasers", JAP, vol. 90, Nu. 4, pg. 1688, 2001.

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