Chapter 5

Discussion

This thesis has demonstrated that the multigrid method can be successfully used to solve the stationary semiconductor equations in one space dimension. The major results of the thesis are summarized in §5.1, while §5.2 discusses some of the ways in which this work can be extended.

5.1 Summary

While straightforward multigrid implementations are not useful for the semiconductor equations, modifications to the basic algorithm produce a successful and efficient program. Changes to the relaxation and prolongation operators had the greatest effect on the convergence rate.

The most successful relaxation scheme is a collective Gauss-Seidel iteration, with the points visited in a symmetric order. Local relaxation sweeps, confined to the neighbourhood of junctions, are effective and inexpensive, and have much the same effect as full iterations do. One iteration of Newton's method can be used to linearize the equations throughout most of the domain, but two iterations should be used near junctions where the solution is rapidly varying.

PROL-1, which is based on the ideas of Algebraic Multigrid and the discrete equations, is the most effective prolongation operator, but PROL-2, which is a cheaper approximation of PROL-1, is a more practical implementation. When combined with local relaxation sweeps, PROL-2 is robust, and greatly improves the convergence of the
algorithm, compared to linear interpolation.

The modified algorithm can be successfully applied to a variety of problems with a wide range of applied potentials. Its performance compares favourably with other multigrid algorithms.

The results of this thesis indicate that the doping profile junctions cause the slow convergence of standard multigrid algorithms. Away from the junctions the solution is well behaved, so the normal multigrid techniques can be expected to be successful, but the interior layers require special treatment, including extra smoothing.

5.2 Suggestions for Future Study

While this thesis has considered only some simple one dimensional problems, this work can form the basis for more extensive studies. Several areas of interest are listed below.

1. For many interesting doping profiles, e.g., thyristors, the solution is not unique and continuation must be used to calculate all solution branches. Continuation techniques are described in [4], for example, and their use in the multigrid context is discussed in [18] and [9].

2. Solving the semiconductor equations in one dimension is useful to isolate the issues involved in applying the multigrid method to the problem, but in practice the equations are usually posed in two or three dimensions. Much of the work of this thesis can be directly extended to multidimensional problems, but some difficulties are expected. These include:

- The symmetric relaxation scheme is successful because information is transmitted in the direction of both $+\nabla \psi$ and $-\nabla \psi$, and in one dimension these directions correspond to either increasing or decreasing $x$. In two or more
dimensions $\nabla \psi$ is not necessarily parallel to a coordinate axis, so the proper relaxation ordering is not obvious.

- The local relaxation sweeps encounter just a few mesh points near the junctions in one dimension, but in larger problems these sweeps will involve larger regions. Block relaxations may need to be used, with the unknowns along a grid line relaxed simultaneously.

- It is not obvious how to extend the prolongations PROL-1 and PROL-2 to multidimensional problems.

Further, the algorithm must be extended to deal with certain aspects of the multidimensional problem (e.g., Neumann boundary conditions) which are not present in the one dimensional case.

3. To adequately resolve the rapid solution changes near the junctions, a nonuniform mesh should be used. Brandt [9] describes a method of incorporating nonuniform grids into the multigrid algorithm by using a hierarchy of uniform grids which do not cover the entire domain. The mesh refinement can be done adaptively, or may follow a prescribed pattern. Some of the issues which may arise are discussed in [13].

4. While only the stationary semiconductor equations have been considered here the transient problem is also of interest. The solution of the time dependent equations involves solving a series of closely related stationary problems; in this way, the transient problem is closely related to continuation. Multigrid algorithms for time dependent problems are discussed in [18] and [9].

5. More insight into the behaviour of the multigrid algorithm can be gained by analyzing the behaviour of the errors. Several assumptions must be made to allow
Local Mode Analysis (LMA) to be applied — the equations must be linearized, and the coefficients must be considered to be fixed or slowly varying. While these assumptions are restrictive, the heuristic analysis may provide guidelines for future developments.