Inverse Doping Profile Analysis for Semiconductor Quality Control

Joseph K. Myers
Faculty: Victor Isakov
Department of Mathematics and Statistics

Abstract. Inverse doping profile problems are linked to inverse conductivity problems under the assumptions of zero space charge and low injection. Unipolar inverse conductivity problems are analyzed theoretically via three uniqueness proofs. Optimized numerical methods are developed for solving the unipolar direct conductivity problem with a piecewise constant conductivity coefficient. Finally, the unipolar inverse conductivity problem is solved for inclusions defined by as many as 9 entirely unknown parameters, or by as many as 120 parameters when an initial guess for each parameter is known with less than 10% error. Our free boundary identification algorithm produces a sequence of improved approximations in a way that provides both regularization and accelerated convergence towards the solution.

1. Introduction
Once upon a time, about one hundred years ago, the properties of semiconductive materials seemed almost like magical powers, and were poorly understood. For instance, beginning in the early history of radio broadcasting, people discovered that “cat's whiskers” had the mysterious ability to drastically improve the reception of radio waves. Just as magnetism was harnessed and compasses superceded celestial navigation, soon semiconductivity would be enlisted as the foot soldier of a technological revolution. Within the length of one human life, mankind would reach the moon, and civilization would become reliant on strange inventions unlike anything in all known world history.

Physicists and mathematicians could not have predicted the changes that would occur in a blink of an eye on history's timescale, but they did see the great potential of semiconductor devices. The electrical conductivity of semiconductors falls between that of conductors (typical conductivities range from 10^4 to 10^6 Siemens per centimeter) and that of insulators (on the order of 10^{-18} to 10^{-10} Siemens per centimeter). This great flexibility in the conductivity of semiconductors, combined with the ability of doping to control the conductivity with great freedom in precisely specified areas, is what makes semiconducting materials so useful. Doping allows devices to be created having a built-to-order doping profile, and thus built-to-order electrical conductivity.

The life of a semiconductor device begins as a pure wafer of undoped silicon substrate. A semiconductor's conductivity is sensitive to minute amounts of impurity atoms. For example, the addition of less than 0.01 percent (one ten-thousandth) of a particular type of impurity can increase the electrical conductivity by four or more orders of magnitude. Carefully-controlled addition of dopants forms a doping profile that regulates electrical conductivity. The result of this doping process is one of 28 common types of semiconductor devices, each with unique characteristics based on their doping profiles.

We wish to determine the doping profile, and thus the function and performance of a semiconductor device, by exterior measurements of electrical voltage and current.

Ultimately, our goal is to provide efficient and accurate testing of semiconductor devices for purposes of quality control, directly at the manufacturing stage and in real-time. So far the theoretical basis has been constructed and successful numerical simulations performed, but experiments in industry remain as future work.

2. Discussion
Calculated quantities of voltage and current, as well as the doping profile, are governed by a complex system of partial differential equations known as the Drift Diffusion Equations [1]. In our research we establish links between drift diffusion and conductivity, which permit us to determine the doping profile by solving the so-called “Inverse Conductivity Problem.” The inverse conductivity problem belongs to a class of mathematical physics problems.

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7 So-called cat’s whiskers were actually primitive versions of Schottkydiodes, a special type of semiconductor diode with a very low forward-voltage drop (resulting in higher efficiency) and a very fast switching action (on the order of one-tenth of one-billionth of one second).

8 Units of conductivity, measured in Siemens, are inversely proportional to units of resistivity, which are measured in ohms.
known as Inverse Problems, which include X-ray tomography, seismic analysis, and image processing. All these problems are very difficult, and in many ways wide open for further mathematical research and analysis, even after decades of continual research by top scientists. For instance, no sonar navigation system is yet able to match the natural navigational ability of a bat, even though both the bat and the submarine’s sonar system are based on the same measurements of reflected sound waves.

Sonar is also the perfect way to understand the goal of an “Inverse Conductivity Problem” in a more familiar way. An algorithm for solving the inverse conductivity problem tries to find an object just as a sonar navigation system would do. The primary distinction is in the data that are used. Instead of sound waves, electrical current and voltage measurements from a long distance away are used to find the location of an unknown object which has disturbed the electro-magnetic field by its presence.

We solve the inverse conductivity problem by expressing its solution as the limit of a minimizing sequence for a functional depending on a parameterized class of direct problems defined in terms of the approximate solutions to the inverse problem, which are initialized by an initial guess consisting of a circle—in the case that no prior information is known—, or a “local” initial guess—when some prior information about the object is known.

![Figure 4: Multi-stage algorithm for locating a nine-parameter domain with one percent noise.](image)

3. Conclusions
We have reduced the stationary drift-diffusion equations into the conductivity equation [2], under reasonable and widely-used assumptions of zero space charge and low injection. The result is a one-to-one relationship between solutions to the inverse problem for the conductivity equation and solutions of the original inverse problem for doping profiles. Then we have proved important global and local uniqueness results for the inverse conductivity problem, as well as a more general class of semilinear elliptic equations. Moreover, we have developed a very efficient and accurate algorithm for solving the direct conductivity problem given in Section 2.7. Finally, we have solved the resulting inverse conductivity problem by finding a minimizing sequence of a suitable error functional, both with and without any initial guess provided.

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5. References