Lecture 1

Overview

Contents

1.1	Introduction	1
1.2	Diffusive electron transport	2
1.3	Types of electron transport	4
1.4	Why study near-equilibrium transport?	6
1.5	About these lectures	6
1.6	Summary	9
1.7	References	9

1.1 Introduction

This short set of lectures is about how electrons in semiconductors and metals flow in response to driving forces such as applied voltages and differences in temperature. The simplest description of transport is the famous Ohm's Law (Georg Ohm, 1927),

$$I = V/R = GV, \qquad (1.1)$$

which states that the current through a conductor is proportional to the voltage across it. One goal of these lectures is to develop an understanding of why and under what conditions the current-voltage characteristic is linear and to understand how the resistance is related to the material properties of the resistor. Before launching into the lectures, let's spend a few minutes discussing what the following lectures are all about.

1.2 Diffusive electron transport

The transport of charge carriers such as electrons is a rich and deep field of physics. While we won't be delving into the underlying physics in great detail, it will be necessary to have a firm grasp of some fundamentals. Consider Fig. 1.1, which illustrates diffusive electron transport in a simple resistor (made with an n-type semiconductor for which the current is carried by electrons in the conduction band).



Fig. 1.1. Illustration of diffusive electron transport in an n-type semiconductor under bias.

Because the positive voltage on the right contact attracts electrons, they tend to flow from left to right, but it is a random walk during which electrons frequently scatter from defects, impurities, etc. In the traditional approach, we say that electrons feel a force due to the electric field,

$$F_e = -q\mathcal{E}_x = qV/L\,.\tag{1.2}$$

The electric field accelerates electrons, but scattering produces an opposing force, so the result is that in the presence of an electric field, electrons drift at a steady-state velocity of

$$v_d = -\mu_n \mathcal{E}_x = \mu_n V/L \,, \tag{1.3}$$

where μ_n is the mobility, a material-dependent parameter.

We obtain the current by noting that it is proportional to the charge on an electron, q, the density of electrons per unit volume, n, the crosssectional area, A, and to the drift velocity, v_d . The current can be written as

$$I = nq\mu_n \frac{A}{L}V = GV, \qquad (1.4)$$

where

$$G = nq\mu_n \frac{A}{L} = \sigma_n \frac{A}{L}, \qquad (1.5)$$

with G being the conductance in Siemens (S = 1/Ohms), and σ_n the conductivity in S/m (1/Ohm-m). Equation (1.4) is a classic result that we shall try to understand more deeply.

Figure 1.2 is a sketch of what a measured I-V characteristic might look like for a semiconductor like silicon. We see that there is a region for which the current varies linearly with voltage. (This is the regime of nearequilibrium, linear, or low-field transport that we shall be concerned with. Under high bias, the current becomes a non-linear function of voltage (and may even be non-monotonic, as in semiconductors like GaAs). A proper discussion of high-field transport would require another set of lecture notes. The interested reader can consult Chapter 7 of Lundstrom [1].

Figure 1.3 illustrates the kind of problem that engineers and applied scientists are increasingly dealing with — an extremely short conductor, in this case a small molecule. The resistance of devices like this can be



Fig. 1.2. Illustration of a typical current vs. voltage characteristic for a semiconductor like silicon.



Fig. 1.3. Illustration of a small organic molecule (phenyl dithiol) attached to two gold contacts. The I-V characteristics of small molecules can now be measured experimentally. See, for example, L. Venkataraman, J. E. Klare, C. Nuckolls, M. S. Hybertsen, and M. L. Steigerwald, "Dependence of single-molecule junction conductance on molecular conformation", *Nature*, **442**, 904-907, 2006.

measured, and we need a theory to understand the measured resistance. Equation (1.4), seems ill-suited to this problem, but a general transport theory should be able to treat both large conductors and very small ones. When we develop this theory, we will find some surprises. For example, we'll find that there is an upper limit to the conductance, no matter how short the conductor is and that conductance comes in quantized units. These facts are well-known from research on mesoscopic physics (e.g. see Datta [2]) but they have now become important in device research and engineering.

1.3 Types of electron transport

Electronic transport is a rich and complex field. Some important types of transport are:

- (1) near-equilibrium transport
- (2) high-field (or hot carrier) transport
- (3) non-local transport in small devices
- (4) quantum transport
- (5) transport in random/disordered/nanostructured materials
- (6) phonon transport

Near-equilibrium transport is diffusive in conductors that are many mean-free-paths long, but it is ballistic when the conductor is much shorter than a mean-free-path. We shall discuss both cases. High field transport in

Overview

bulk semiconductors is also diffusive, but since the carriers gain significant kinetic energy from the high electric field, they are more energetic (hotter) than the lattice. Under high applied biases, the current is a nonlinear function of the applied voltage, and Ohm's Law no longer holds. (See Chapter 7 of Lundstrom [1] for a discussion of high field transport.)

In modern semiconductor devices, modest applied biases (e.g. 1 V) can produce large electric fields across the short, active regions. Under these conditions, carrier transport becomes a nonlocal function of the electric field, and interesting effects such as velocity overshoot can occur. (See Chapter 8 of Lundstrom [1] for a discussion of these effects.) Finally, as devices get very short and the potential changes rapidly on the scale of the electron's wavelength, effects like quantum mechanical reflection and tunneling become important. For an introduction to the field of quantum tranport, see Datta [3].

Another important class of problems has to do with transport in various kinds of disordered materials. Much of traditional transport theory assumes a periodic crystal lattice and makes use of concepts like crystal momentum and Brillouin zones. In these lectures, we will restrict our attention to this class of problems. Amorphous materials, however, do not possess long range order; some interesting new features occur, but many of the essential aspects of scattering are similar (e.g. see Mott and Davis [4]). Polycrystalline materials consist of single crystal grains separated by grain boundaries. The statistical distributions of grain sizes, orientations, and grain boundary properties complicate the description of electron transport. Indeed, much of the promise of nanotechnology lies in the hope that artificially structuring matter at the nanoscale will provide properties not found in nature. We believe that the approach used in these lectures will prove useful for this class of problems as well, but this is a topic of current research, and the lecture notes volume will have to wait.

Finally, we should mention that although our attention in these lectures is on electron transport in semiconductors and metals. Phonon transport is also important, and many of the concepts developed to describe electron transport can just as well describe phonon transport. The calculation of the thermal conductivity is much like the calculation of the electrical conductivity. Just as for electrons, there can be near-equilibrium, diffusive, ballistic, far-from-equilibrium, and quantum (or wave-like) transport of phonons in crystalline or disordered materials. In modern integrated circuits, power dissipation from electron transport heats the lattice and generates phonons. Understanding how to manage this problem requires us to understand both electron and phonon transport. The performance of thermoelectric devices used for electronic cooling and for electrical power generation from thermal gradients is controlled by both electron and phonon transport. Although our focus in these lectures is on electron transport, a brief discussion of phonon transport is also included.

1.4 Why study near-equilibrium transport?

Given that near-equilibrium transport in crystalline materials is only a small subset of carrier transport, one might question the need to devote an entire volume to the topic. There are some good reasons. First, nearequilibrium transport is the foundation for understanding transport in general. Concepts introduced in the study of near-equilibrium are often extended to treat more complicated problems, and near-equilibrium transport provides a reference point for comparison when we analyze transport in more complex situations. Second, near-equilibrium transport measurements are extensively used to characterize electronic materials and to understand the properties of new materials. Finally, near-equilibrium transport controls or strongly influences the performance of most electronic devices.

There is a very large number of books that discuss low-field transport from a traditional perspective — typically using the Boltzmann Transport Equation (e.g. see Refs. [5-7]). In this volume, I use a new approach that I believe is more physically transparent, mathematically more simple, and that is more broadly applicable.

1.5 About these lectures

The list of lectures presented in this collection is:

- Lecture 1: Overview
- Lecture 2: General Model for Transport
- Lecture 3: Resistance: Ballistic to Diffusive
- Lecture 4: Thermoelectric Effects: Physical Approach
- Lecture 5: Thermoelectric Effects: Mathematics
- Lecture 6: An Introduction to Scattering
- Lecture 7: Boltzmann Transport Equation
- Lecture 8: Near-equilibrium Transport: Measurements
- Lecture 9: Phonon Transport

Lecture 10: Graphene: A Case Study

A brief description of each of these lectures follows.

Lecture 2: General Model for Transport

Datta's model of a nanodevice (a version of the Landauer approach) [8] is introduced as a general way to describe transport in nanodevices — as well as in bulk metals and semiconductors.

Lecture 3: Resistance: Ballistic to Diffusive

The resistance of a ballistic conductor and concepts such as the quantum contact resistance are introduced and discussed. The results are then generalized to treat transport all the way from the ballistic to diffusive regimes. We will show how to treat bulk conductors (electrons free to move in 3D) and will also discuss 2D conductors (electrons free to move in a plane) and 1D conductors (electrons free to move along a wire).

Lecture 4: Thermoelectric Effects: Physical Approach

The effect of temperature gradients on current flow and how electrical currents produce heat currents will be discussed. Coupled equations for the electric and heat currents will be presented, and applications to electronic cooling and the generation of electrical power from thermal gradients will be briefly discussed. In this lecture, we use a physical approach and try to keep the mathematics to a minimum.

Lecture 5: Thermoelectric Effects: Mathematics

Beginning with the general model for transport, we mathematically derive expressions for the four thermoelectric transport coefficients:

- (i) Electrical conductivity
- (ii) Seebeck coefficient (or "thermopower")
- (iii) Peltier coefficient
- (iv) Electronic heat conductivity

We also discuss the relationship of the coefficients (e.g. the Kelvin relation and the Wiedemann-Franz Law).

Lecture 6: An Introduction to Scattering

In Lectures 1-5, scattering is described by a mean-free-path (MFP) for backscattering. In this lecture, we show how the MFP is related to the time between scattering events and briefly discuss how the scattering time is related to underlying physical processes.

Lecture 7: Boltzmann Transport Equation

Semi-classical carrier transport is traditionally described by the Boltzmann Transport Equation (BTE) (e.g. [1, 5-7]). In this lecture, we present the BTE, show how it is solved, and relate it to the Landauer approach used in these lectures. As an example of the use of the BTE, we derive the conductivity in the presence of an applied *B*-field.

Lecture 8: Near-equilibrium Transport: Measurements

Measurements of near-equilibrium transport are routinely used to characterize electronic materials. This lecture is a brief introduction to commonlyused techniques such as van der Pauw and Hall effect measurements.

Lecture 9: Phonon Transport

Most of the heat flow in semiconductors is carried by phonons (i.e. quantized lattice vibrations). In the presence of a small temperature gradient, phonon transport is also a problem in near-equilibrium transport, and the techniques developed for electron transport can be readily extended to phonons. This lecture is an introduction to phonon transport. Key similarities and differences between electron and phonon transport are discussed.

Lecture 10: Graphene: A Case Study

In Lectures 1-8 we largely consider applications of near-equilibrium electron transport to traditional materials, such as semiconductors with parabolic

energy bands, but the theory is much more general. As an example of how to apply the concepts in these lectures, we discuss near-equilibrium transport in graphene, a material that has recently attracted a lot of attention and was the subject of the 2010 Nobel Prize in Physics.

Appendix: Brief Summary of Key Results

The central ideas conveyed in these notes are easy to grasp, but the notes contain many equations so that the reader can see all the steps in the derivations of key results. To assist the reader in performing computations, the key results are summarized in this short appendix, which includes pointers to specific results in the various lectures. Expressions of the four transport parameters for materials with simple bandstructures are often needed and are also listed in this appendix.

1.6 Summary

My objectives for this collection of lectures are very simple:

- (1) To introduce the essentials of near-equilibrium carrier transport using a "bottom up" approach that works at the nanoscale as well as at the macroscale.
- (2) To acquaint students with some key results (e.g. the quantum of conductance, common measurement techniques).
- (3) To provide a basic foundation upon which students can build as they encounter problems in research and engineering.

Your goal in reading these lecture notes should be to acquire a firm understanding of the fundamental concepts and to develop an ability to apply these fundamentals to real problems. Those interested in developing a deeper understanding of the physics of transport should consult Refs. [2, 3, 8].

1.7 References

For an introduction to high-field transport and to non-local transport in semiconductor devices, see Chapters 7 and 8 in:

 Mark Lundstrom, Fundamentals of Carrier Transport 2nd Ed., Cambridge Univ. Press, Cambridge, U.K., 2000.

Chapters 1 and 2 in the following book are a good introduction to the socalled Landauer approach.

[2] Supriyo Datta, *Electronic Transport in Mesoscopic Systems*, Cambridge Univ. Press, Cambridge, U.K., 1995.

For an introduction to quantum transport, see:

[3] Supriyo Datta, Quantum Transport: Atom to transistor, Cambridge Univ. Press, Cambridge, U.K., 2005.

For a classic introduction to electronic conduction in noncrystalline materials, see:

[4] N.F. Mott and E.A. Davis, *Electronic Processes in Non-Crystalline Ma*terials, Clarendon Press, Oxford, U.K., 1971.

Three classic references on low-field transport are:

- [5] J.M. Ziman, *Principles of the Theory of Solids*, Cambridge Univ. Press, Cambridge, U.K., 1964.
- [6] A.C. Smith, J. Janak, and R. Adler, *Electronic Conduction in Solids*, McGraw-Hill, New York, N.Y. 1965.
- [7] N.W. Ashcroft and N.D. Mermin, *Solid–State Physics*, Saunders College, Philadelphia, PA, 1976.

The conceptual approach used in these lectures is presented in a succinct form by Datta:

[8] Supriyo Datta, Lessons from Nanoelectronics: A new approach to transport theory, World Scientific Publishing Company, Singapore, 2011.

- A collection of additional resources on carrier transport can be found at:
- [9] Mark Lundstrom and Supriyo Datta, "Electronics from the Bottom Up", http://nanohub.org/topics/ElectronicsFromTheBottomUp, 2011.

Hear a lecture on this chapter at:

[10] M. Lundstrom, "General Model for Transport", http://nanohub.org/ topics/LessonsfromNanoscience, 2011.