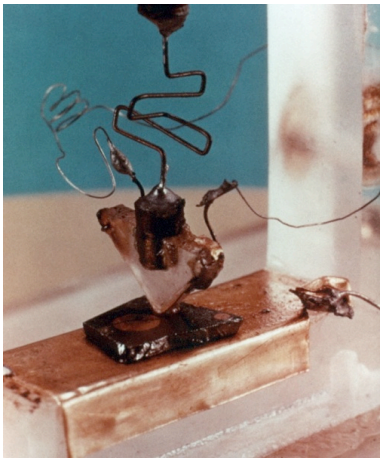
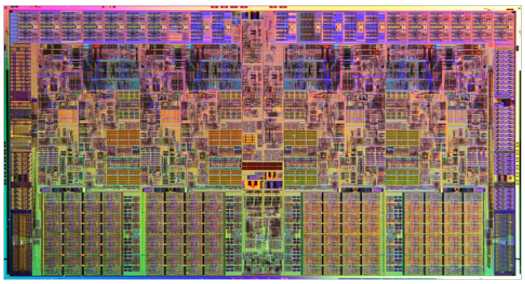
Lecture 8 Drude (Classical) Theory of Electrons in Metals

Reading: Simon: Ch 3, also see extra reading on duo from Ashcroft and Mermin

We have seen a rapid development in the performance of electronic devices in the last 50 years. This has been achieved through a detailed understanding of the properties of electrons in crystalline systems.

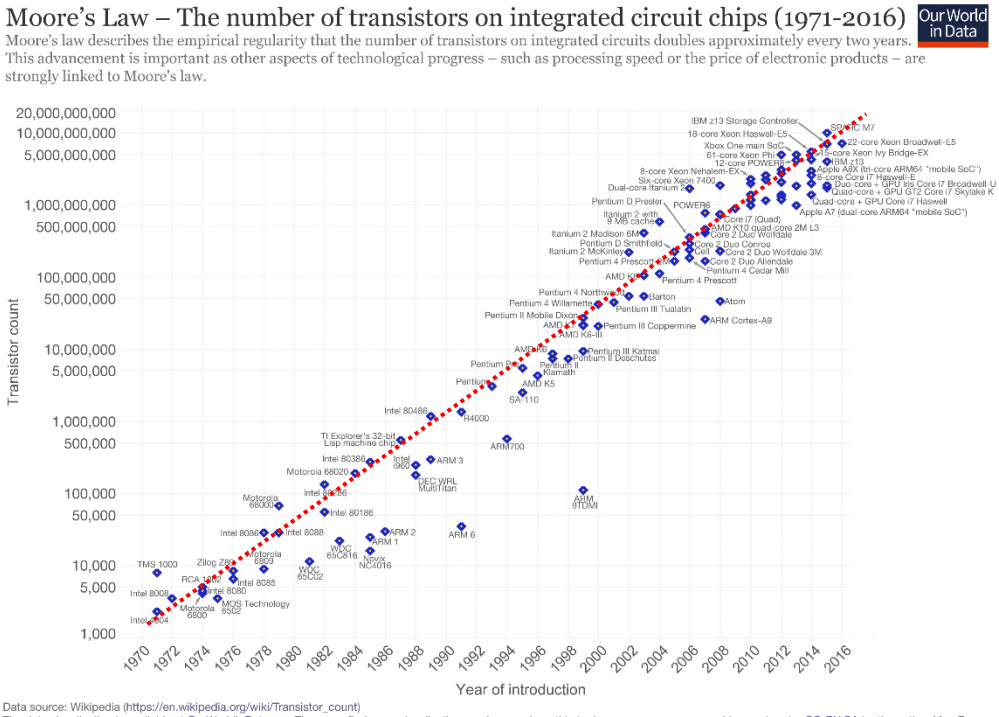


The first transistor – Bell laboratories 1947. This is based on the semiconductor germanium. Its development took 10 years of research.



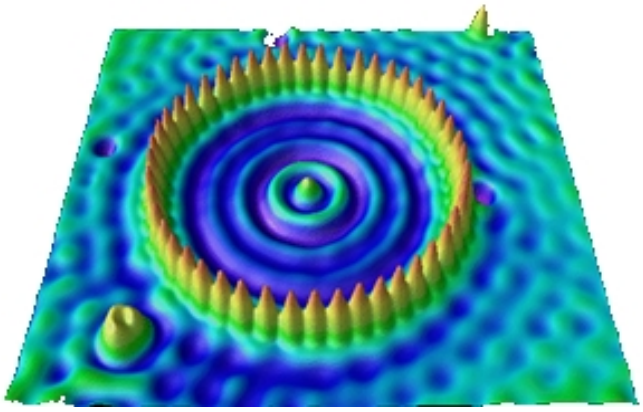
Intel Core i7 processor. (2010). Approximately the same size as the first transistor. Contains 730 million transistors, each with dimensions ~45 nm

The development of electronic devices has followed an empirical law – Moore's law.



Moore's law states that the number of transistors in an integrated circuit will double every two years.

Leading research today:



48 Fe atoms assembled with a scanning tunnelling microscope STM on a Cu(111) surface

Electrons in Solids

We start our consideration of electrons in solids by exploring a *classical model* of electrons in metals.

Metals comprise a significant class of materials (over 2/3 of the periodic table).

Common properties of all metals are:

- Conduct electricity
- Conduct heat
- Ductile
- Shiny when freshly exposed to air

We require a theory to understand all these properties.

First model – theory of metallic conduction proposed by Drude in 1900 (3 years after discovery of electron in 1897). This model is not covered in Kittel, however it is significant enough to warrant one lecture.

Recommended text Ashcroft and Mermin Chapter 1. (See additional reading material on duo for a copy of this chapter.)

Drude model was entirely classical yet it had some remarkable successes, however it also has major limitations.

Drude model give an insight into the electrical properties of crystalline solids. The problems with the Drude model were only resolved after the development of quantum mechanics and a quantum theory of solids.

Drude constructed the model by applying the kinetic theory of gases to metals which he considered as a “gas of electrons”.

In simple gases there is only one type of particle present. Drude realised that there must be at least 2 types of particle in a metal as electrons are negatively charged and the metal is electrically neutral.

Drude assumed that this positive charge was in heavier, immobile particles.

Two assumptions are made:

1. The outer (valence) electrons become detached from atoms and move freely around the metal. They behave as a classical gas of particles with charge -|e| and mass m_e.
2. Electric fields due to negative electrons and positive ions cancel on average and can be ignored. This can be further broken down into the two approximations we consider today: ignore ions: free electron, ignore other electrons: independent electron.

In a metal the core electrons remain bound to the nucleus forming the ion. The valence electrons move more freely throughout the crystal – these are sometime referred to as conduction electrons.

Drude applied kinetic theory to the gas of conduction electrons mass m_e which move freely amongst heavy immobile ions.

Some predictions of the Drude model:

1. Specific heat capacity of electrons

(We remember that phonons also have a heat capacity, leave aside at present).
The mean kinetic energy of a classical particle at a temperature *T* is

$$E_{\mathrm{ke}} = \frac{3}{2} k_{\mathrm{B}} T$$

(remember k_{B} is Boltzmann's constant and $k_{\mathrm{B}} = R/N_{\mathrm{A}}$)

We recall that this is an example of the equipartition theorem.

The specific heat capacity of each electron is given by:

$$C_{\mathrm{V}} = \frac{dE_{\mathrm{ke}}}{dT} = \frac{3}{2} k_{\mathrm{B}}$$

This is *independent* of temperature.

The total electronic heat capacity per unit volume is given by nC_{V} where n is the valence electron density per unit volume (m^{-3}).

Experimentally we observe that the heat capacity is much smaller and is proportional to T.

2. Electrical conductivity
We begin with Ohms law, the current flowing along a wire *I* is proportional to the potential drop along the wire *V* = *IR*.

We can rewrite this to eliminate the dimensions, or size, of the system being considered: $E = \rho J$
where *E* is electric field (V m^{-1}), *ρ* is resistivity (Ω m). *J* current density (A m^{-2}).
Can also write this as $J = \sigma E$ where *σ* is electrical conductivity (1/*ρ*).

Further assumptions in the Drude model are collisions occur between electrons and other electrons or ions. These collisions are instantaneous events which abruptly

alter the velocity of the electron. (Think about physical mechanism of resistance – electron collisions)

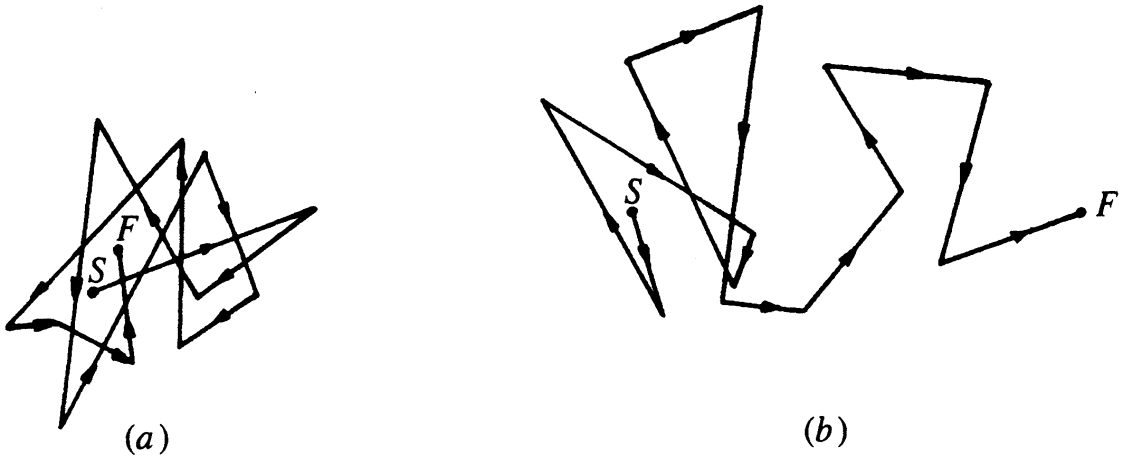
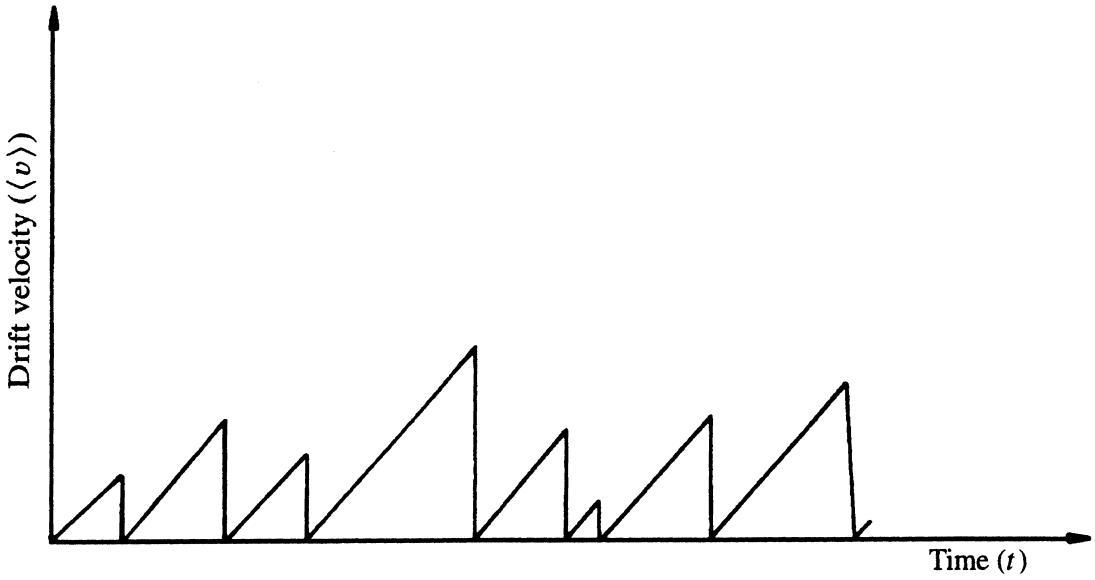


Figure illustrating drift velocity. (a) zero electric field, (b) finite electric field. In an electric field the start and finish positions differ – leading to a net flow of current.



Variation of drift velocity under an electric field. The average time between collisions is τ. The picture illustrates the assumption that collisions randomise the motion and the velocity starts again from zero.

Drude thought that electron-ion collisions were more important. (This is actually not the case as electron-electron collisions have a bigger effect.)

The average time between collision events is τ the relaxation time.

In the absence of an electric field the random nature of the motion produces an average velocity $\underline{v}$ of zero – resulting in no net current flow.

When an electric field is present $\underline{E}$ there will be a mean electronic velocity in the opposite direction to the field. This is called the *Drift velocity*.

We can calculate this by considering an electron at a time *t* after the previous collision. If the velocity immediately after the collision was v_0 then the velocity at time *t* will be

$$\underline{v} = \underline{v_0} - \frac{|e|t\underline{E}}{m_e}$$

We assume that the electron direction is random following a collision then there will be no contribution from $\underline{v_0}$ to the average electronic velocity

The electron velocity must therefore be given by the average of the $-\frac{|e|t\underline{E}}{m_e}$

$$\underline{v}_{\text{ave}} = -\frac{|e|t_{\text{ave}}\underline{E}}{m_e} \quad \text{where } t_{\text{ave}} = \tau$$

Current flow is given by

$$\underline{J} = -n|e|v$$

$$\underline{J} = \frac{n|e|^2\tau}{m_e}\underline{E}$$

$$\sigma = \frac{n|e|^2\tau}{m_e}$$

This is the Drude conductivity formula; we have used τ as the symbol for the average collision time.

This can be used with limitations to describe the electrical conductivity of a range of metals. For metals at room temperature τ is typically 10^{-14} - 10^{-15} seconds.

Is this a reasonable number? To answer consider the mean distance between collisions and use $l = v_0\tau$ where v_0 is the average electronic speed. Drude estimated v_0 from the classical equipartition theorem:

$$\frac{1}{2}mv_0^2 = \frac{3}{2}k_{\text{B}}T$$

This gives $v_0 = 10^5$ ms^{-1} at room temperature and the mean free path is then l = 0.1-1 nm which is comparable to the atom spacing. We can see where Drude got his idea of the importance of electron-ion collisions.

We will show later that this classical estimate of v_0 at room temperature is wrong by about a factor of 10.

Further calculations may be performed with the Drude model without any knowledge of the details of the collision mechanism being known.

3. Thermal conductivity of electrons

Using the Drude model we can determine the rate at which electrons can carry heat through a metal. If we consider a temperature gradient dT/dz, then thermal energy will be transported along the temperature gradient in the opposite direction to the gradient from high to low temperatures. The thermal energy carried by an electron will depend on the temperature at the point where it experiences its last collision. The assumption is that each electron collision results in the electrons having the

same thermal energy as the lattice at the point of collision, as defined by the temperature at that point.

The rate at which electrons carry excess heat per unit area past a point in the metal is given by Q = - electron density × electron *z* velocity × heat capacity per electron × *z* distance travelled since last collision × temperature gradient.

$$Q = -nv_z C_V v_z \tau \frac{dT}{dz}$$

The negative sign signifies that the hottest electrons will move in the direction of decreasing temperature.

The thermal average of $v_z^2 = \frac{k_B T}{m_e}$ so that we have

$$Q = -n\frac{k_B}{m_e} T C_V \tau \frac{dT}{dz}$$

The thermal conductivity is defined by $Q = -\kappa \frac{dT}{dz}$ symbol κ

Substituting our earlier value for $C_V = \frac{3}{2} k_B$ we finally get

$$\kappa = \frac{3}{2} n \frac{k_B^2 T}{m_e} \tau$$

The Wiedemann-Franz Law

This was an empirical law developed by Wiedemann and Franz in 1853.

It stated that the ratio of the thermal conductivity to electrical conductivity for a range of metals is directly proportional to the temperature where the proportionality constant is roughly the same for all metals.

Using the Drude model we get

$$\frac{\kappa}{\sigma} = \frac{3}{2}\left(\frac{k_B}{e}\right)^2 T$$

Where $\frac{\kappa}{\sigma T} = 1.11 \times 10^{-8}$ W Ω K^{-2}

This is about half the value observed in experiment.

EXPERIMENTAL THERMAL CONDUCTIVITIES AND LORENZ NUMBERS OF SELECTED METALS

ELEMENT	273 K		373 K	
	κ (watt/cm-K)	$\kappa/\sigma T$ (watt-ohm/K^2)	κ (watt/cm-K)	$\kappa/\sigma T$ (watt-ohm/K^2)
Li	0.71	2.22×10^{-8}	0.73	2.43×10^{-8}
Na	1.38	2.12		
K	1.0	2.23		
Rb	0.6	2.42		
Cu	3.85	2.20	3.82	2.29
Ag	4.18	2.31	4.17	2.38
Au	3.1	2.32	3.1	2.36
Be	2.3	2.36	1.7	2.42
Mg	1.5	2.14	1.5	2.25
Nb	0.52	2.90	0.54	2.78
Fe	0.80	2.61	0.73	2.88
Zn	1.13	2.28	1.1	2.30
Cd	1.0	2.49	1.0	
Al	2.38	2.14	2.30	2.19
In	0.88	2.58	0.80	2.60
Tl	0.5	2.75	0.45	2.75
Sn	0.64	2.48	0.60	2.54
Pb	0.38	2.64	0.35	2.53
Bi	0.09	3.53	0.08	3.35
Sb	0.18	2.57	0.17	2.69

Ashcroft and Mermin Table 1.6

The Drude model was remarkably successful in predicting the Wiedemann-Franz law (to within a factor of two). It treats electrons in metals as classical particles. This was one of the greatest successes of the Drude model. Its seeming success however, was due to two factors which roughly cancel.

At room temperature the electronic contribution to the specific heat is ~100 times smaller than predicted by the Drude model and the mean square electron speed is ~100 times larger. It was rather a lucky coincidence.

A correct treatment of electrons in crystals requires a quantum treatment.