

# HW1 solution

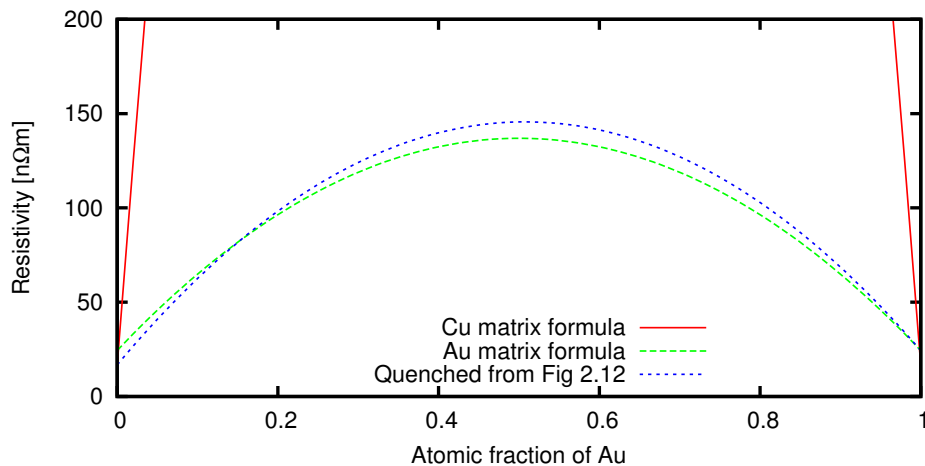
MTLE-6120: Spring 2019

Due: Jan 21, 2019

## 1. Resistivity of Cu-Au alloys

Read section 2.3.2 of Kasap and pay particular attention to Figure 2.12. The resistivity of alloys varies with atomic fraction  $X$  as  $\rho = \rho_{\text{matrix}} + CX(1 - X)$ , where  $C$  is called the Nordheim coefficient. For Cu-Au alloys, for small Cu fractions in Au,  $\rho_{\text{matrix}} \equiv \rho_{\text{Cu}}$ , and for small Au fractions  $\rho_{\text{matrix}} = \rho_{\text{Au}}$ .

- (a) At 20° C,  $\rho_{\text{Cu}} = 16.8 \text{ n}\Omega\text{m}$  and  $\rho_{\text{Au}} = 24.4 \text{ n}\Omega\text{m}$ . For dilute alloys,  $C_{\text{Au in Cu}} = 5500 \text{ n}\Omega\text{m}$  and  $C_{\text{Cu in Au}} = 450 \text{ n}\Omega\text{m}$ . Plot the resistivity as a function of Au atom fraction in Cu, all the way from  $X = 0$  (pure copper) to  $X = 1$  (pure gold) using both the Cu and Au matrix formulae. Compare these two plots to the ‘Quenched’ line from Figure 2.12 in Kasap and explain.



Using the Cu in Au matrix agrees well on the entire composition range, but the Au in Cu does not.  $C$  is defined for dilute alloys, so it need not be applicable for all concentrations. This comparison indicates that dilute limit of Au in Cu behaves very differently from other concentrations.

- (b) Using the Cu in Au matrix formula, estimate the temperature coefficient of resistivity of the 50-50 (quenched) Cu-Au alloy and contrast it to that of the pure metals,  $\alpha_{\text{Au}} = 0.0034 \text{ K}^{-1}$  and  $\alpha_{\text{Cu}} = 0.0039 \text{ K}^{-1}$ .

At  $X = 0.5$ ,  $\rho = \rho_{\text{Au}} + 0.25C_{\text{Cu in Au}}$ . The  $\rho_{\text{Au}}$  part is due to thermal scattering and is temperature dependent (approximately linear in  $T$  as discussed in class). The mixing part is due to impurities and is approximately constant in  $T$ . Therefore:

$$\begin{aligned} \frac{d\rho}{dT} &= \frac{d}{dT} (\rho_{\text{Au}} + 0.25C_{\text{Cu in Au}}) \\ &= \frac{d\rho_{\text{Au}}}{dT} \\ \alpha &\equiv \frac{d\rho}{\rho dT} \\ &= \frac{\frac{d\rho_{\text{Au}}}{dT}}{\rho_{\text{Au}} + 0.25C_{\text{Cu in Au}}} \end{aligned}$$

$$\begin{aligned}
&= \frac{\frac{d\rho_{\text{Au}}}{\rho_{\text{Au}}dT}}{1 + \frac{0.25C_{\text{Cu in Au}}}{\rho_{\text{Au}}}} \\
&= \frac{\alpha_{\text{Au}}}{1 + \frac{0.25C_{\text{Cu in Au}}}{\rho_{\text{Au}}}} \\
&= \frac{0.0034\text{K}^{-1}}{1 + \frac{0.25 \cdot 450}{24.4}} \\
&= 0.00061\text{K}^{-1}
\end{aligned}$$

The temperature coefficient of the alloy is much smaller because the scattering is dominated by impurities, a temperature-independent contribution. This fact, along with the overall higher resistivity, is the reason why resistive wires are usually made of alloys eg. nichrome and constantan.

- (c) From the Nordheim coefficients, calculate the cross-sections  $\sigma_{\text{Au in Cu}}$  of electron scattering against Au impurities in Cu and  $\sigma_{\text{Cu in Au}}$  of electron scattering against Cu impurities in Au. Assume that the electron velocity is approximately  $v_F = 1.5 \times 10^6$  m/s in both cases. (Notation warning:  $\sigma$  is the standard symbol both for scattering cross section and conductivity.)

The cross-section  $\sigma_{\text{ion}}$  determines the mean-free path  $\lambda = 1/(n_{\text{ion}}\sigma_{\text{ion}})$ , where  $n_{\text{ion}}$  is the number density of the ion. In the case of impurities,  $n_{\text{ion}} = Xn_{\text{matrix}}$ , where  $n_{\text{matrix}}$  is the number density of ions in the pure matrix. So we have

$$\lambda^{-1} = Xn_{\text{matrix}}\sigma_{\text{ion}}$$

The resistivity is

$$\begin{aligned}
\rho &\equiv \sigma^{-1} = \frac{m}{ne^2\tau} && \text{(Drude conductivity)} \\
&= \frac{m}{ne^2} (\tau_T^{-1} + \tau_I^{-1}) && \text{(Mathiessen's rule)} \\
&= \frac{m}{ne^2} (v_F\lambda_T^{-1} + v_F\lambda_I^{-1}) \\
&= \frac{mv_F}{ne^2} (\lambda_T^{-1} + Xn_{\text{matrix}}\sigma_{\text{ion}}) \\
&= \rho_{\text{matrix}} + CX && \text{(dilute limit, where } X \ll 1) \\
\Rightarrow C &= \frac{mv_F}{ne^2} n_{\text{matrix}}\sigma_{\text{ion}} \\
&= \frac{mv_F\sigma_{\text{ion}}}{e^2} && \text{(one electron per ion for Cu and Au } \Rightarrow n_{\text{matrix}} = n) \\
\Rightarrow \sigma_{\text{ion}} &= \frac{Ce^2}{mv_F}
\end{aligned}$$

All values on RHS are now known, and we can substitute:

$$\begin{aligned}
\sigma_{\text{Au in Cu}} &= \frac{C_{\text{Au in Cu}}e^2}{mv_F} = \frac{5500 \times 10^{-9}\Omega\text{m} \cdot (1.6 \times 10^{-19}\text{C})^2}{9 \times 10^{-31}\text{kg} \cdot 1.5 \times 10^6\text{m/s}} = 1.04 \times 10^{-19} \text{ m}^2 = 10.4 \text{ \AA}^2 \\
\sigma_{\text{Cu in Au}} &= \frac{C_{\text{Cu in Au}}e^2}{mv_F} = \frac{450 \times 10^{-9}\Omega\text{m} \cdot (1.6 \times 10^{-19}\text{C})^2}{9 \times 10^{-31}\text{kg} \cdot 1.5 \times 10^6\text{m/s}} = 8.5 \times 10^{-21} \text{ m}^2 = 0.85 \text{ \AA}^2
\end{aligned}$$

- (d) Hypothesize why  $\sigma_{\text{Au in Cu}} \gg \sigma_{\text{Cu in Au}}$ , and why the dilute Au in Cu limit is so different from other concentrations.

Cu atoms are smaller than Au atoms, with Cu metal having a 10% smaller lattice constant. Cu impurities in Au can 'fit' in the lattice easily, whereas Au impurities in Cu have to push the

surrounding Au atoms. Thus, electrons scattering against Cu in Au are effectively only scattering against the impurity, whereas for Au in Cu, the electrons are scattering against the impurity and also the surrounding atoms that have been displaced (strain field), thereby increasing the cross section for scattering.

This effect is expected for low concentrations when you can think of one metal as an impurity in the other. At higher concentrations, the overall lattice constant itself changes, and surrounding atom displacement is not as necessary.

## 2. Damped harmonic oscillator differential equation

This problem should help you revise / get comfortable solving ordinary differential equations and working with Fourier transforms.

- (a) Find the general solution of the homogeneous differential equation

$$m\ddot{x}(t) - \gamma\dot{x}(t) + kx(t) = 0$$

where  $\dot{x}(t) \equiv dx(t)/dt$ . Hint: try solutions of the form  $x(t) = Ae^{iwt}$ , find all  $w$  for which  $A \neq 0$  (non-trivial solutions), and the general solution is the linear combination of all such solutions.

Substitute  $x(t) = Ae^{iwt}$  into the differential equation to find

$$-mw^2 Ae^{iwt} - i\gamma w Ae^{iwt} + kAe^{iwt} = 0.$$

For a solution with  $A \neq 0$ , one therefore needs to satisfy

$$-mw^2 - i\gamma w + k = 0,$$

which is a quadratic with solutions

$$w_{\pm} = \frac{i\gamma}{2m} \pm \sqrt{\frac{k}{m} - \left(\frac{\gamma}{2m}\right)^2}.$$

The general solution is therefore

$$x(t) = A_+ e^{iw_+ t} + A_- e^{iw_- t}$$

with  $w_{\pm}$  as solved above.

- (b) Find the specific solution of the previous differential equation that satisfies initial conditions  $x(0) = x_0$  and  $\dot{x}(0) = 0$ .

Substituting the general solution into the two initial conditions yields.

$$\begin{aligned} x_0 = x(0) &= A_+ + A_-, \\ 0 = \dot{x}(0) &= iw_+ A_+ + iw_- A_-. \end{aligned}$$

Solving the simultaneous equations,

$$\begin{aligned} A_+ &= \frac{w_- x_0}{w_- - w_+}, \\ A_- &= \frac{w_+ x_0}{w_+ - w_-}. \end{aligned}$$

so that (defining  $\omega_0 \equiv \sqrt{\frac{k}{m} - \left(\frac{\gamma}{2m}\right)^2}$  and  $\Gamma \equiv \frac{\gamma}{2m}$  for convenience)

$$\begin{aligned} x(t) &= x_0 \frac{w_- e^{iw_+ t} - w_+ e^{iw_- t}}{w_- - w_+} \\ &= x_0 \frac{(i\Gamma - \omega_0) e^{i(i\Gamma + \omega_0)t} - (i\Gamma + \omega_0) e^{i(i\Gamma - \omega_0)t}}{-2\omega_0} \end{aligned}$$

$$\begin{aligned}
&= x_0 \frac{i\Gamma e^{(-\Gamma+i\omega_0)t} - \omega_0 e^{(-\Gamma+i\omega_0)t} - i\Gamma e^{(-\Gamma-i\omega_0)t} - \omega_0 e^{(-\Gamma-i\omega_0)t}}{-2\omega_0} \\
&= x_0 \cos(\omega_0 t) e^{-\Gamma t} + x_0 \frac{\Gamma}{\omega_0} \sin(\omega_0 t) e^{-\Gamma t}.
\end{aligned}$$

Note that if  $\gamma \rightarrow 0$  i.e.  $\Gamma \rightarrow 0$ , the solution  $x(t) = x_0 \cos(\omega_0 t)$  oscillates forever at the natural frequency  $\omega_0$ . But damping  $\gamma$  causes the solution to decay, eventually leading to  $x(t) \rightarrow 0$  as  $t \rightarrow \infty$ .

- (c) Find the general solution of the forced harmonic oscillator

$$m\ddot{x}(t) - \gamma\dot{x}(t) + kx(t) = Fe^{-i\omega t}.$$

What is the ‘steady-state’ solution for large times  $t \gg m/\gamma$ ? Hint: the general solution of an inhomogeneous equation is that of the corresponding homogeneous equation + a particular solution  $x_p(t)$ ; in this case, try  $x_p(t) = x_1 e^{-i\omega t}$ .

Substitute the particular solution  $x_p(t) = x_1 e^{-i\omega t}$  into the differential equation to get

$$-m\omega^2 x_1 e^{-i\omega t} + i\gamma\omega x_1 e^{-i\omega t} + kx_1 e^{-i\omega t} = Fe^{-i\omega t},$$

which yields

$$x_1 = \frac{F}{-m\omega^2 + i\gamma\omega + k} = \frac{F}{m(-\omega^2 + 2i\Gamma\omega + \omega_0^2)}.$$

The general solution is therefore

$$\begin{aligned}
x(t) &= A_+ e^{i\omega_+ t} + A_- e^{i\omega_- t} + x_p(t) \\
&= A_+ e^{(-\Gamma+i\omega_0)t} + A_- e^{(-\Gamma-i\omega_0)t} + \frac{Fe^{-i\omega t}}{m(-\omega^2 + 2i\Gamma\omega + \omega_0^2)} \\
&= (A_+ e^{i\omega_0 t} + A_- e^{-i\omega_0 t}) e^{-\Gamma t} + \frac{Fe^{-i\omega t}}{m(-\omega^2 + 2i\Gamma\omega + \omega_0^2)}.
\end{aligned}$$

For a given boundary condition, we will have to solve for  $A_{\pm}$  as before, but note that part always decays to zero as  $t \rightarrow \infty$ . The steady state solution is just the particular solution

$$x(t \gg \Gamma^{-1}) \approx \frac{Fe^{-i\omega t}}{m(-\omega^2 + 2i\Gamma\omega + \omega_0^2)}.$$

- (d) Show that the steady-state solution above can be easily ‘solved in the Fourier domain’ by assuming  $x(t) = x e^{-i\omega t}$  and replacing  $d/dt \rightarrow -i\omega$  in the differential equation.

That is exactly how we obtained the particular solution, which is the steady-state solution.

### 3. Optical response of bound electrons

In class, we solved the equation of motion of a free electron to derive Drude theory. Now consider the opposite limit, where electrons are tightly bound to atoms, which is the most reasonable classical description for electrons in insulating materials. Specifically, assume that each electron is attached to an atom with spring constant  $k$  and damping constant  $\gamma$ , that is if it is displaced by  $\vec{r}(t)$ , there will be a restoring force  $-k\vec{r}(t)$  and damping force  $-\gamma \frac{d\vec{r}}{dt}$ .

- (a) Solve the equation of motion for an electrons position  $\vec{r}(t)$ , when an oscillatory electric field  $\vec{E}(t) = \vec{E} e^{-i\omega t}$  is applied. What is the induced dipole moment  $\vec{p}$  due to this electron? (Hint: this is extremely easy in the frequency domain, as set up by the previous problem.)

The net force on the electron is due to the electric field, restoring and damping forces. Hence

$$m \frac{d^2 \vec{r}(t)}{dt^2} = -e\vec{E} e^{-i\omega t} - k\vec{r}(t) - \gamma \frac{d\vec{r}}{dt}$$

Substituting  $\vec{r}(t) = \vec{r}e^{-i\omega t}$  (where  $\vec{r}$  is a constant amplitude) yields

$$\begin{aligned} m\vec{r}\frac{d^2e^{-i\omega t}}{dt^2} &= -e\vec{E}e^{-i\omega t} - k\vec{r}e^{-i\omega t} - \gamma\vec{r}\frac{de^{-i\omega t}}{dt} \\ -m\vec{r}\omega^2 &= -e\vec{E} - k\vec{r} + i\omega\gamma\vec{r} \\ (k - m\omega^2 - i\omega\gamma)\vec{r} &= -e\vec{E} \\ \vec{r} &= \frac{-e\vec{E}}{k - m\omega^2 - i\omega\gamma} \end{aligned}$$

The induced dipole moment due to the oscillating electron is

$$\begin{aligned} \vec{p} &= (-e)\vec{r} \\ &= \frac{e^2\vec{E}}{k - m\omega^2 - i\omega\gamma} \end{aligned}$$

Note that this is the amplitude for an oscillating dipole  $\vec{p}(t) = \vec{p}e^{-i\omega t}$ .

- (b) Assume that there is a number density  $n_b$  of such bound electrons that all respond the same way as above. Calculate the polarization  $\vec{P}$ , displacement field  $\vec{D}$ , and hence the dielectric function  $\epsilon(\omega)$ .

$$\begin{aligned} \vec{P} &= n\vec{p} \\ &= \frac{n_b e^2}{k - m\omega^2 - i\omega\gamma} \vec{E} \\ \vec{D} &\equiv \epsilon_0 \vec{E} + \vec{P} \\ &= \left( \epsilon_0 + \frac{n_b e^2}{k - m\omega^2 - i\omega\gamma} \right) \vec{E} \\ \epsilon(\omega) &= \epsilon_0 + \frac{n_b e^2}{k - m\omega^2 - i\omega\gamma} \end{aligned}$$

- (c) Express the dielectric function in terms of the spring resonant frequency  $\omega_0 = \sqrt{k/m}$  and damping rate  $\Gamma = \gamma/m$ , and the plasma frequency of bound electrons  $\omega_{pb} = \sqrt{n_b e^2 / (m\epsilon_0)}$ . How does this differ from the Drude result for free electrons?

Substituting  $k = m\omega_0^2$  and  $\gamma = m\Gamma$  in previous result yields

$$\begin{aligned} \epsilon(\omega) &= \epsilon_0 + \frac{n_b e^2}{k - m\omega^2 - i\omega\gamma} \\ &= \epsilon_0 + \frac{n_b e^2}{m\omega_0^2 - m\omega^2 - im\omega\Gamma} \\ &= \epsilon_0 + \frac{n_b e^2/m}{\omega_0^2 - \omega^2 - i\omega\Gamma} \\ &= \epsilon_0 + \frac{\omega_{pb}^2 \epsilon_0}{\omega_0^2 - \omega^2 - i\omega\Gamma} \\ &= \epsilon_0 \left( 1 + \frac{\omega_{pb}^2}{\omega_0^2 - \omega^2 - i\omega\Gamma} \right) \end{aligned}$$

If you take  $\omega_0 \rightarrow 0$  and set  $\Gamma = \tau^{-1}$ , this becomes the Drude formula. Basically, taking the resonant frequency to zero makes the spring constant vanish, freeing the electron! Damping of the spring corresponds exactly to losses due to scattering. This generalized form is called the Drude-Lorentz model.

- (d) In a real metal, some electrons are free and the rest are bound to the atoms. In copper, for example, 1 s electron per atom is effectively free, while 10 d electrons are bound tightly to the atoms. (The remaining ‘core’ electrons are bound so tightly that we can assume exactly fixed, and ignore them.) Write the dielectric function for this general case with  $n$  free electrons and  $n_b$  spring-bound electrons.

The contributions due to the two types of electrons simply add in the polarization and yield

$$\epsilon(\omega) = \epsilon_0 \left( 1 - \underbrace{\frac{\omega_p^2}{\omega^2 + i\omega/\tau}}_{\text{Drude (free)}} + \underbrace{\frac{\omega_{pb}^2}{\omega_0^2 - \omega^2 - i\omega\Gamma}}_{\text{Spring-bound}} \right)$$

where it is just important to distinguish that there are two different plasma frequencies,  $\omega_p^2 = ne^2/(m\epsilon_0)$  for the Drude free electrons and  $\omega_{pb}^2 = n_b e^2/(m\epsilon_0)$  for the spring-bound electrons. Also, the scattering rate  $\tau^{-1}$  for the free electrons will be different from the damping rate  $\Gamma$  for the spring bound electrons.