4.12 Density of states in a band   Consider the density of states function in Equation 4.10. By substituting the units for each variable and by using suitable interrelations between units, show that the units for $g(E)$ is $J^{-1}\ m^{-3}$.

Solution

$$g(E) = (8\pi 2^{1/2})\left(\frac{m_e}{h^2}\right)^{3/2} E^{1/2} \rightarrow \left[\frac{(kg)}{(Js)^2}\right]^{3/2} (J)^{1/2} \rightarrow \frac{(kg)^{3/2}}{(Js)^3}(J)^{1/2} \rightarrow \frac{(kg)^{3/2}}{(J)^{5/2}(s)^3} \rightarrow \frac{(kg)^{3/2}}{(J)^{5/2}(s)^3}$$

$$g(E) \rightarrow \frac{(kg)^{3/2}}{(J)(J)^{3/2}(s)^3} \rightarrow \frac{(kg)^{3/2}(m)^3}{(J)(m)^3(J)^{3/2}(s)^3} \rightarrow \frac{1}{(J)(m)^3}\cdot\frac{(kg)^{3/2}(m)^3}{(J)^{3/2}(s)^3} \rightarrow \frac{1}{(J)(m)^3}\cdot\frac{(kg)^{3/2}(m)^3}{(m^2\,kg\,s^{-2})^{3/2}(s)^3}$$

where we have used   Energy (J) = force (N) × distance (m) = mass (kg) × acceleration (m s⁻²) × distance (m) =   (kg)(m s⁻²)(m) =   (kg)(m² s⁻²). Thus,

$$g(E) \rightarrow \frac{1}{(J)(m)^3}\cdot\frac{(kg)^{3/2}(m)^3}{(m^2\,kg\,s^{-2})^{3/2}(s)^3} \rightarrow \frac{1}{(J)(m)^3}\cdot\frac{(kg)^{3/2}(m)^3}{(m)^3(kg)^{3/2}(s^{-3})(s)^3} \rightarrow \frac{1}{(J)(m)^3}$$

4.13   Fermi-Dirac distribution   Consider the Fermi-Dirac function, $f(E) = 1/[e^{(E-E_F)/kT}+1]$. Define $x = (E - E_F)/kT$ and hence show that $f'(x) = df(x)/dx = -e^x/(e^x + 1)^2$. (a) Plot $f(x)$ vs. x and $y = |f'(x)/f'(0)|$ vs. x. (b) What are f and y at $x = \pm 2$? What does the interval $\Delta x = 4$ about $x = 0$ represent? (c)   Show that the width Δx of the y vs. x curve between the $y = 0.1$ values is approximately 7.2. (d) What are your conclusions?

Solution

$$\therefore \qquad v_{\text{thermal}} = \sqrt{\frac{3Tk}{m_e}} = \sqrt{\frac{3(293 \text{ K})(1.381 \times 10^{-23} \text{ J/K})}{(9.109 \times 10^{-31} \text{ kg})}}$$

$\therefore \qquad$ **$v_{\text{thermal}} = 1.15 \times 10^5$ m/s**

Comparing the two values:

$\qquad$ **Ratio** $= v_F / v_{\text{thermal}} = $ **13.7**

$\qquad v_F$ is about 14 times greater than v_{thermal}. This is because v_{thermal} assumes that electrons do not interact (more states than electrons) and obey Maxwell-Boltzmann statistics ($E_{av} = 3/2kT$). However, in a metal there are many conduction electrons (comparable to the total number of states). They interact with the metal ions and obey the Pauli exclusion principle, i.e. Fermi-Dirac statistics. They extend to higher energies to avoid each other and thereby fulfill the Pauli exclusion principle.

b. The De Broglie wavelength is $\lambda = h/p$ where $p = m_e v_F$ is the momentum of the electrons.

$$\lambda = \frac{h}{m_e v_F} = \frac{6.626 \times 10^{-34} \text{ J s}}{(9.109 \times 10^{-31} \text{ kg})(1.57 \times 10^6 \text{ m/s})}$$

$\therefore \qquad$ **$\lambda = 4.63 \times 10^{-10}$ m** or **4.63 Å**

The interplanar separation, d, is given as 2.09 Å. The diffraction condition is:

$$\lambda = 2d\sin\theta$$

$$\therefore \qquad \sin\theta = \frac{1}{2}\frac{\lambda}{d} = \frac{1}{2}\frac{(4.63 \text{ Å})}{(2.09 \text{ Å})} = 1.11$$

Since this is greater than 1, and $\sin\theta$ cannot be greater than 1, the electrons will not be diffracted.

c. The drift mobility is related to the mean scattering time τ by:

$$\tau = \frac{\mu m_e}{e} = \frac{(33 \times 10^{-4} \text{ m}^2 \text{ V}^{-1} \text{ s}^{-1})(9.109 \times 10^{-31} \text{ kg})}{1.602 \times 10^{-19} \text{ C}} = 1.876 \times 10^{-14} \text{ s}$$

The mean free path, λ_F, of electrons with speed, v_F is:

$\qquad \lambda_F = v_F \tau = (1.57 \times 10^6 \text{ m/s})(1.876 \times 10^{-14} \text{ s}) = $ **2.95×10^{-8} m** or **295 Å**

The mean free path of those electrons with effective speeds v_e (close to mean speed) can be found as follows (E_F exhibits very little change with temperature, therefore $E_F \approx E_{FO}$):

$$\frac{1}{2}m_e v_e^2 = \frac{3}{5}E_{FO} = \frac{3}{5}E_F$$

$$\therefore \qquad v_e = \sqrt{\frac{6}{5}\frac{E_F}{m_e}} = \sqrt{\frac{6}{5}\frac{(7.0 \text{ eV})(1.602 \times 10^{-19} \text{ J/eV})}{(9.109 \times 10^{-19} \text{ kg})}} = 1.215 \times 10^6 \text{ m/s}$$

$\therefore \qquad \lambda_e = v_e \tau = (1.215 \times 10^6 \text{ m/s})(1.876 \times 10^{-14} \text{ s}) = $ **2.28×10^{-8} m** or **228 Å**

4.15 Free electron model, Fermi energy, and density of states Na and Au both are valency I metals; that is, each atom donates one electron to the sea of conduction electrons. Calculate the Fermi

energy (in eV) of each at 300 K and 0 K. Calculate the mean speed of all the conduction electrons and also the speed of electrons at E_F for each metal. Calculate the density of states as states per eV cm^{-3} at the Fermi energy.

Solution

Since Na and Au are valency I metal, their electron concentrations, n are then the atomic concentrations multiplied by the group number, or:

$$n_{Na} = (\text{Valency})\frac{N_A d_{Na}}{M_{Na}} = (1)\frac{(6.022 \times 10^{23}\, \text{mol}^{-1})(968\, \text{kgm}^{-3})}{23 \times 10^{-3}\, \text{kg/mol}} = 2.53 \times 10^{28}\, \text{m}^{-3}$$

$$n_{Au} = (\text{Valency})\frac{N_A d_{Au}}{M_{Au}} = (1)\frac{(6.022 \times 10^{23}\, \text{mol}^{-1})(19300\, \text{kgm}^{-3})}{197 \times 10^{-3}\, \text{kg/mol}} = 5.9 \times 10^{28}\, \text{m}^{-3}$$

At 0 K,

$$E_{FO}(\text{Na}) = \frac{h^2}{8m_e}\left(\frac{3n}{\pi}\right)^{\frac{2}{3}} = \frac{(6.626 \times 10^{-34}\, \text{J s})^2}{8 \times 9.1 \times 10^{-31}\, \text{kg}}\left(\frac{3 \times 2.53 \times 10^{28}\, \text{m}^{-3}}{\pi}\right)^{2/3}$$

$$= \mathbf{5.04 \times 10^{-19}\ J\ or\ 3.15\ eV}$$

$$= \mathbf{8.863 \times 10^{-19}\ J\ or\ 5.54\ eV}$$

At 300 K,

$$E_F(\text{Na}) = E_{FO}(\text{Na})\left[1 - \frac{\pi^2}{12}\left(\frac{kT}{E_{FO}(\text{Na})}\right)^2\right] = 3.15\text{eV}\left[1 - \frac{\pi^2}{12}\left(\frac{0.02585\text{eV}}{3.15\text{eV}}\right)^2\right]$$

∴ $E_F(\text{Na}) = \mathbf{3.15\ eV}$

$$E_F(\text{Au}) = E_{FO}(\text{Au})\left[1 - \frac{\pi^2}{12}\left(\frac{kT}{E_{FO}(\text{Au})}\right)^2\right] = 5.54\text{eV}\left[1 - \frac{\pi^2}{12}\left(\frac{0.02585\text{eV}}{5.54\text{eV}}\right)^2\right]$$

∴ $E_F(\text{Au}) = \mathbf{5.54\ eV}$

Mean speed v_e of conduction electrons (sometimes also called the *effective* speed) can be found from

$$\frac{1}{2}m_e v_e^2 = E_{average} = \frac{3}{5}E_{FO}$$

∴ $v_e = (6E_{FO}/5m_e)^{1/2}$

∴ $v_e(\text{Na}) = (6E_{FO}(\text{Na})/5m_e)^{1/2} = ((6 \times 3.15 \times 1.6 \times 10^{-19}\, \text{J})/(5 \times 9.1 \times 10^{-31}\text{kg}))^{1/2}$

∴ $v_e(\text{Na}) = \mathbf{8.15 \times 10^5\ ms^{-1}}$

and $v_e(\text{Au}) = (6E_{FO}(\text{Au})/5m_e)^{1/2} = ((6 \times 5.54 \times 1.6 \times 10^{-19}\, \text{J})/(5 \times 9.1 \times 10^{-31}\text{kg}))^{1/2}$

∴ $v_e(\text{Au}) = \mathbf{1.08 \times 10^6\ ms^{-1}}$

Speed at E_F is given by

$$\frac{1}{2}m_e v_F^2 = E_{FO}$$

$\therefore$ $v_F = (2E_{FO}/m_e)^{1/2}$

$\therefore$ $v_F(\text{Na}) = (2E_{F0}(\text{Na})/m_e)^{1/2} = ((2\times3.15\times1.6\times10^{-19}\text{ J})/(9.1\times10^{-31}\text{kg}))^{1/2}$

$\therefore$ $v_F(\text{Na}) = \mathbf{1.05\times10^6\ ms^{-1}}$

and $v_F(\text{Au}) = (2E_{F0}(\text{Au})/m_e)^{1/2} = ((2\times5.54\times1.6\times10^{-19}\text{ J})/(9.1\times10^{-31}\text{kg}))^{1/2}$

$\therefore$ $v_F(\text{Au}) = \mathbf{1.4\times10^6\ ms^{-1}}$

The density of states is given by

$$g(E) = (8\pi 2^{1/2})\left(\frac{m_e}{h^2}\right)^{3/2} E^{1/2}$$

For Na, $g_{E_F}(\text{Na}) = (8\pi 2^{1/2})\left[\dfrac{9.1\times10^{-31}\text{kg}}{6.626\times10^{-34}\text{ Js}}\right]^{3/2}(3.15\times1.6\times10^{-19}\text{ J})^{1/2}$

$\therefore$ $g_{E_F}(\text{Na}) = 7.54\times10^{46}\text{ m}^{-3}\text{J}^{-1} = (7.54\times10^{46}\text{ m}^{-3}\text{J}^{-1})(10^{-6}\text{ m}^3\text{cm}^{-3})(1.6\times10^{-19}\text{ JeV}^{-1})$

$= \mathbf{1.2\times10^{22}\ cm^{-3}\ eV^{-1}}$

For Au, $g_{E_F}(\text{Au}) = (8\pi 2^{1/2})\left[\dfrac{9.1\times10^{-31}\text{kg}}{6.626\times10^{-34}\text{ Js}}\right]^{3/2}(5.54\times1.6\times10^{-19}\text{ J})^{1/2}$

$\therefore$ $g_{E_F}(\text{Au}) = 10\times10^{46}\text{ m}^{-3}\text{J}^{-1} = (10\times10^{46}\text{ m}^{-3}\text{J}^{-1})(10^{-6}\text{ m}^3\text{cm}^{-3})(1.6\times10^{-19}\text{ JeV}^{-1})$

$= \mathbf{1.6\times10^{22}\ cm^{-3}\ eV^{-1}}$

Notice the similarity in the magnitudes of the density of states at the Fermi energy.

4.16 Fermi energy and electron concentration   Consider the metals in Table 4.9 from groups I, II and III in the Periodic Table. Calculate the Fermi energies at absolute zero, and compare the values with the experimental values. What is your conclusion?

Table 4.9

Metal	Group	M_{at}	Density (g cm^{-3})	E_F(eV) [Calculated]	E_F(eV) [Experiment]
Cu	I	63.55	8.96	—	6.5
Zn	II	65.38	7.14	—	11.0
Al	III	27	2.70	—	11.8

Solution

Since Cu is in group I, its valency is also 1. The electron concentration n is then the atomic concentration multiplied by the group number, or:

$$n = (\text{Valency})\frac{N_A D}{M_{at}} = (1)\frac{(6.022\times10^{23}\text{ mol}^{-1})(8.96\times10^3\text{ kg/m}^3)}{63.55\times10^{-3}\text{ kg/mol}} = 8.490\times10^{28}\text{ m}^{-3}$$

the Fermi energy at 0 K from Equation 4.22 is

$$E_{FO}(\text{eV}) = \frac{h^2}{8m_e}\left(\frac{3n}{\pi}\right)^{\frac{2}{3}}\left(\frac{1}{e}\right)$$

$\therefore$
$$E_{FO} = \frac{(6.626\times10^{-34}\text{ J s})^2}{8(9.109\times10^{-31}\text{ kg})}\left(\frac{3(8.490\times10^{28}\text{ m}^{-3})}{\pi}\right)^{\frac{2}{3}}\left(\frac{1}{1.602\times10^{-19}\text{ J/eV}}\right)$$

$\therefore$ **E_{FO} = 7.04 eV**

Comparing with the experimental value:

$$|\%\text{ difference}| = \left|\frac{7.04\text{ eV} - 6.5\text{ eV}}{6.5\text{ eV}}\right| \times 100\% = \textbf{8.31\%}$$

E_{FO} can be calculated for Zn and Al in the same way (remember to take into account the different valencies). The values are summarized in the following table and it can be seen that calculated values are close to experimental values:

Table 4Q16-1: Summarized values for Fermi energy at absolute zero temperature.

Metal	n (m^{-3}) ($\times$ 10^{28})	E_{FO} (eV) (calculated)	E_F (eV) (experimental)	% Difference
Cu	8.490	**7.04**	6.5	**8.3**
Zn	13.15	**9.43**	11.0	**14.3**
Al	18.07	**11.7**	11.8	**0.85**

Author's Note: The experimental values for the Fermi energy are only approximate (±0.5 eV). For Al and Cu they have been extracted from soft x-ray emission spectra. For Zn, E_F is from low temperature heat capacity measurements which generates an effective mass of 0.85 (see comment above on Table 4.2), and the latter corresponds to $E_F = 11$ eV.   Further information may be found in the following references (there are many others).

Aluminum: W.M. Cady and D.H. Tomboulian, *Phys. Rev.,* **59***,* 381, 1941; O. Aita and T. Sagawa, J. Phys. Soc. Jpn, **27**, 164, 1969; J.C. Fuggle et al. *Phys. Rev. B*, **16**, 75, 1977

Copper: C.S. Fadley and D.A. Shirley, *Journal of Research of the Notional Bureau of Standards* - A. Physics and Chemistry, **74A** (No. 4), 543, 1970 (Figure 9, p552)

Zinc: L.G. Parrat, *Rev. Mod. Phys.*, **31**, 616, 1959 as soft x-ray spectra which indicate a very rough value ~12 eV. (It is generally quite difficult to get a clean Zn surface of x-ray photoelectron spectroscopy.) Zn effective mass in Table 4.2 is used for generating an experimental E_F in Table 4.9. It represents what E_F should be from low-temperature heat capacity measurements.

4.17 Temperature dependence of the Fermi energy

a.   Given that the Fermi energy for Cu is 7.0 eV at absolute zero, calculate the E_F at 300 K. What is the percentage change in E_F and what is your conclusion?

b.   Given the Fermi energy for Cu at absolute zero, calculate the average energy and mean speed per conduction electron at absolute zero and 300 K, and comment.

Solution

a. The Fermi energy in eV at 0 K is given as 7.0 eV. The temperature dependence of E_F is given by Equation 4.23. Remember that E_{FO} is given in eV.

$$E_F = E_{FO}\left(1 - \frac{\pi^2}{12}\left[\frac{kT}{E_{FO}}\right]^2\right)$$

$\therefore$ $$E_F = (7.0\,\text{eV})\left(1 - \frac{\pi^2}{12}\left[\frac{(1.381 \times 10^{-23}\,\text{J/K})(300\,\text{K})}{(7.0\,\text{eV})(1.602 \times 10^{-19}\,\text{J/eV})}\right]^2\right) = \textbf{6.999921 eV}$$

$\therefore$ $$\left|\%\,\textbf{difference}\right| = \left|\frac{6.999921\,\text{eV} - 7.0\,\text{eV}}{7.0\,\text{eV}}\right| \times 100\% = \textbf{0.00129\%}$$

This is a very small change. The Fermi energy appears to be almost unaffected by temperature.

b. The average energy per electron at 0 K is:

$$\textbf{\textit{E}}_\textbf{av}\textbf{(0 K)} = 3/5\ (E_{FO}) = \textbf{4.2 eV}$$

The average energy at 300 K can be calculated from Equation 4.26:

$$E_{av}(T) = \frac{3}{5}E_{FO}\left(1 + \frac{5\pi^2}{12}\left[\frac{kT}{E_{FO}}\right]^2\right)$$

$\therefore$ $$E_{av}(300\,\text{K}) = \frac{3}{5}(7.0\,\text{eV})\left(1 + \frac{5\pi^2}{12}\left[\frac{(1.381 \times 10^{-23}\,\text{J/K})(300\,\text{K})}{(7.0\,\text{eV})(1.602 \times 10^{-19}\,\text{J/eV})}\right]^2\right)$$

$\therefore$ $$\textbf{\textit{E}}_\textbf{av}\textbf{(300 K)} = \textbf{4.200236 eV}$$

This is a very small change.

Assume that the mean speed will be close to the effective speed v_e. Effective speed at absolute zero is denoted as v_{eo}, and is given by:

$$E_{av}(0\,\text{K}) \times q = \frac{1}{2}m_e v_{eo}{}^2$$

$\therefore$ $$v_{eo} = \sqrt{2\frac{qE_{av}(0\,\text{K})}{m_e}} = \sqrt{2\frac{(1.602 \times 10^{-19}\,\text{J/eV})(4.2\,\text{eV})}{(9.109 \times 10^{-31}\,\text{kg})}} = \textbf{1,215,446 m/s}$$

At 300 K, the effective speed is v_e:

$$v_e = \sqrt{2\frac{qE_{av}(300\,\text{K})}{m_e}} = \sqrt{2\frac{(1.602 \times 10^{-19}\,\text{J/eV})(4.200236\,\text{eV})}{(9.109 \times 10^{-31}\,\text{kg})}} = \textbf{1,215,480 m/s}$$

Comparing the values:

$$|\% \text{ difference}| = \left| \frac{12,154,80 \text{ m/s} - 12,15,446 \text{ m/s}}{12,15,446 \text{ m/s}} \right| \times 100\% = \mathbf{0.0028\%}$$

The mean speed has increased by a negligible amount (0.003%) from 0 K to 300 K.

Note: For thermal conduction, this tiny increase in the velocity is sufficient to transport energy from hot regions to cold regions. This very small increase in the velocity also allows the electrons in many metals to diffuse from hot to cold regions giving rise to the Seebeck effect (with cold side negative).

4.18 Fermi energy in Mg The density and atomic mass of Mg are 1.74 g cm^{-3}, and 24.31 g mol^{-1}. Mg is in Group II in the Periodic Table. Calculate the Fermi energy of the electrons in Mg in eV to two decimal places. When a Mg target is bombarded by electrons in a vacuum tube, soft x-ray are emitted whose spectra are shown in Table 4.10 in two rows at a time as photon energy *hf* (eV) and relative intensity *I,* where the maximum value of *I* has been assigned 100. Plot *I* vs. *hf*. Plot also *I/f^3* vs. *hf*, but with maximum *I/f^3* set to 100. What is your conclusion? The reason for dividing *I* by *f^3* is that the emitted x-ray intensity is proportional to two factors: (a) the concentration of electrons n_E at *E* that can fall down to the vacated *L*-shell, and (b) a quantum mechanical probability transition probability that depends on $(hf)^3$.

Table 4.10 Soft x-ray emission data from a magnesium target in an x-ray tube. Electron bombardment of the target knocks out *L*-shell electrons. Conduction electrons fall down in energy and fill the vacated *L*-states.

hf (eV)	39.5	40	40.5	41	41.5	42	42.5	43	43.5	44
I	0.57	0.70	1.12	2.45	3.99	6.26	11.0	18.1	27.1	37.4
hf (eV)	44.5	45	45.5	46	46.5	47	47.5	48	48.4	48.8
I	48.4	57.7	64.5	70.7	75.6	79.8	82.4	83.2	81.4	85.4
hf (eV)	48.9	49	49.1	49.2	49.3	49.4	49.5	49.6	50	50.4
I	90.9	96.4	100.0	83.5	43.5	15.3	7.48	4.02	1.16	0.43

Data extracted from Table I in W.M. Cady and D.H. Tomboulian, *Phys. Rev.* **57**, 381, 1941.

Solution

Since Mg is in group II, its valency is also 2. The electron concentration *n* is then the atomic concentration multiplied by the group number, or:
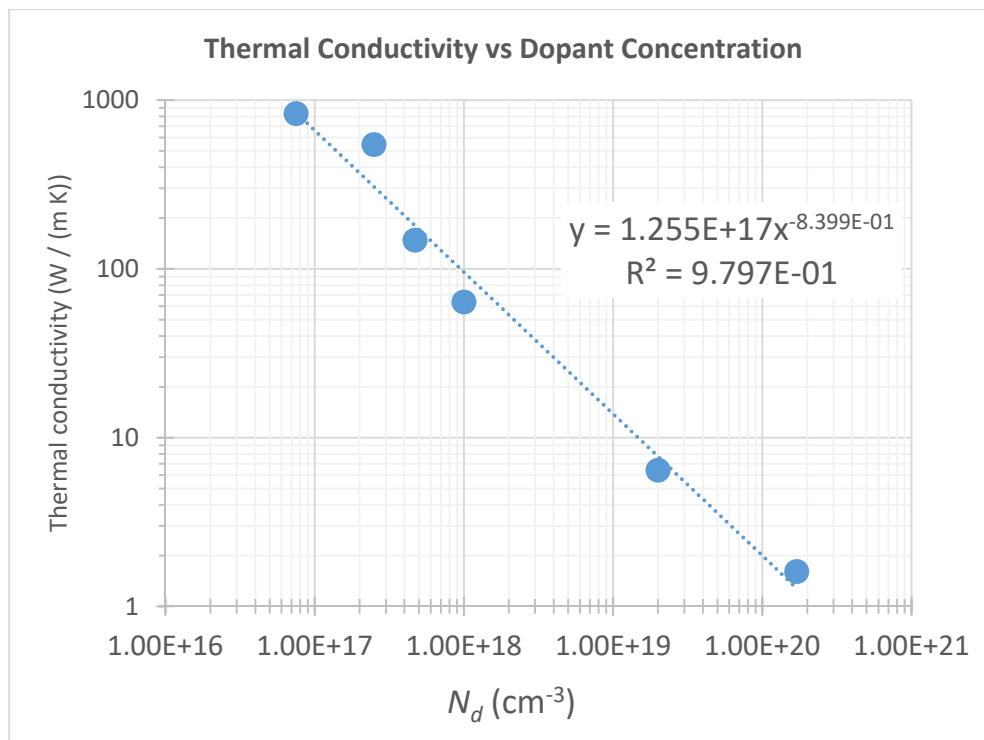
$$n = (\text{Valency}) \frac{N_A \rho}{M_{at}} = (2) \frac{(6.022 \times 10^{23} \text{ mol}^{-1})(1.74 \times 10^3 \text{ kg/m}^3)}{24.31 \times 10^{-3} \text{ kg/mol}} = 8.621 \times 10^{28} \text{ m}^{-3}$$

The Fermi energy at 0 K is

$$E_{FO}(\text{eV}) = \frac{h^2}{8m_e} \left(\frac{3n}{\pi} \right)^{\frac{2}{3}} \left(\frac{1}{e} \right)$$

$$\therefore \quad E_{FO} = \frac{(6.626 \times 10^{-34} \text{ J s})^2}{8(9.109 \times 10^{-31} \text{ kg})} \left(\frac{3(8.621 \times 10^{28} \text{ m}^{-3})}{\pi} \right)^{\frac{2}{3}} \left(\frac{1}{1.602 \times 10^{-19} \text{ J/eV}} \right)$$

$$\therefore \qquad \mathbf{\mathit{E_{FO}} = 7.1 \text{ eV}}$$

Figure 4Q39-1 The log-log plot of thermal conductivity of a silicon single crystal vs dopant concentration, κ vs. N_d. The best power law dependence is also shown. All data points at 10 K. Data from Table 4.18.

We can use the arguments in 4Q38 that, at low temperatures, the phonon concentration is low so that impurities play an important role in scattering the phonons in a doped crystal. κ depends on the mean free path λ of the phonons. If we neglect all other phonon scattering processes, then the phonon mean free path would be determined by the dopant (impurity) concentration N_d. A phonon travels a distance λ and then it is scattered by a dopant. If S is the cross sectional area of the dopant, then in the volume $S\lambda$ there must be at least 1 dopant, that is $S\lambda N_d = 1$. Thus,

$$\kappa \propto \lambda = \frac{1}{SN_d} \tag{1}$$

The experimental results in Figure 4Q39-1 approximately follow the above behavior. Recall that we neglected all other phonon scattering processes in Equation (1), so we should not expect an exact agreement.

Author's Note: At sufficiently lower dopant concentrations, κ loses its dependence on N_d as other scattering mechanisms (phonon-phono, crystal defects, surfaces) dominate. See D. Fortier, K. Suzuki. "Effect of P-donors on thermal phonon scattering in silicon", *Journal de Physique*, 1976, **37** (2), 143-147.

*4.40 Overlapping bands   Consider Cu and Ni with their density of states as schematically sketched in Figure 4.61. Both have overlapping 3*d* and 4*s* bands, but the 3*d* band is very narrow compared to the 4*s* band. In the case of Cu the band is full, whereas in Ni, it is only partially filled.

a. In Cu, do the electrons in the 3*d* band contribute to electrical conduction? Explain.

b. In Ni, do electrons in both bands contribute to conduction? Explain.

c. Do electrons have the same effective mass in the two bands? Explain.

d. Can an electron in the 4*s* band with energy around E_F become scattered into the 3*d* band as a result of a scattering process? Consider both metals.

e. Scattering of electrons from the 4*s* band to the 3*d* band and vice versa can be viewed as an additional scattering process. How would you expect the resistivity of Ni to compare with that of Cu, even though Ni has two valence electrons and nearly the same density as Cu? In which case would you expect a stronger temperature dependence for the resistivity?
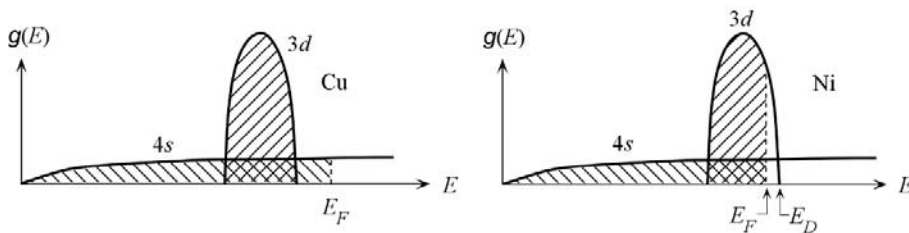
Figure 4.68 Density of states and electron filling in Cu and Ni

Solution

a. In Cu the 3*d* band is full, so the electrons in this band do not contribute to conduction.

b. In Ni both the 3*d* and 4*s* bands are partially filled so electrons in both bands can gain energy from the field and move to higher energy levels. Thus both contribute to electrical conductivity.

c. No, because the effective mass depends on how easily the electron can gain energy from the field and accelerate or move to higher energy levels. The energy distributions in the two bands are different. In the 4*s* band, the concentration of states is increasing with energy whereas in the 3*d* band, it is decreasing with energy. One would therefore expect different inertial resistances to acceleration, different effective mass and hence different drift mobility for electrons in these bands.

d. Not in copper because the 3*d* band is full and cannot take electrons. In Ni the electrons can indeed be scattered from one band to the other, e.g. an electron in the 4*s* band can be scattered into the 3*d* band. Its mobility will then change. Electrons in the 3*d* band are very sluggish (low drift mobility) and contribute less to the conductivity.

e. Ni should be more resistive because of the additional scattering mechanism from the 4*s* to the 3*d* band (Matthiessen's rule). This scattering is called *s-d* scattering. One may at first think that this *s-d* scattering de-emphasizes the importance of scattering from lattice vibrations and hence, overall, the resistivity should be less temperature dependent. In reality, electrons in Ni also get scattered by magnetic interactions with Ni ion magnetic moments (Nickel is ferromagnetic; Ch. 8 in the textbook) which has a stronger temperature dependence than $\rho \sim T$.

4.41 Overlapping bands at E_F and higher resistivity Figure 4.61 shows the density of states for Cu (or Ag) and Ni (or Pd). The *d*-band in Cu is filled and only electrons at E_F in the *s* band make a contribution to the conductivity. In Ni, on the other hand, there are electrons at E_F both in the *s* and *d* bands. The *d* band is narrow compared with the *s* band, and the electron's effective mass in this *d* band