PROBLEMS

5.1 Calculate the electron density needed to produce the first crossover in Fig. 5.21. What would the charge density have to be for the first crossover to occur between the second and third nearest neighbors of iron (a_{Fe} = 2.86Å).

5.2 Describe and contrast the valence electronic structure and magnetic characteristics of

i) free iron atoms
ii) atoms in metallic iron
iii) iron ions in magnetic Fe_3O_4

5.3 Explain what happens as copper is alloyed with nickel, $Ni_{1-x}Cu_x$. Describe the valence electronic structure and the magnetic moment in terms of a simple band model. Be quantitative where possible.

5.4 Calculate the effect on the total energy of an alloy as states in a flat *d*-band are filled.

5.5 Verify Eqs. 5.7 and 5.9.

5.6 a) Explain why ferromagnetism is observed in nickel $(4s\ 3d)^{10}$ but not in titanium $(4s\ 3d)^4$.

b) Explain why ferromagnetism is observed in the metals of the 3*d* transition series and not in the metals of the 3*p* series (e.g. Al).

5.7 You are running a billion dollar a year specialty steel operation. You want to improve the corrosion resistance of a magnetic iron alloy but do not want the saturation magnetization to decrease too much. While talking in your office to an old classmate you receive a phone call that you can buy several tons of either Mg or Ti at a bargain price. All you know is that Mg has a positive heat of formation with iron (+20 kJ/mole) and Ti has a negative heat of formation (-26 kJ/mole).

a) If both are equally effective in improving corrosion resistance, which would you buy?

b) If you can justify your choice to your colleague, perhaps even impressing him with your knowledge of the Pauli exclusion principle, he may nominate you to be a fellow of the American Physical Society. What do you tell him?

5.8 a) Use your understanding of the electronic structure of metals to explain the general parabolic trend and the magnetic exceptions to that trend shown in Figs. 5.20 a and b. While answering this question be sure to

- sketch representative electronic state densities,
- explain the relation between atomic volume and bulk modulus,
- discuss the relation between electron kinetic energy and atomic volume,

b) Estimate the fractional volume change in Fe due to its magnetic moment and give a numerical value for the pressure needed to cause such a volume change. Discuss the possible relation of this effect to the structure Fe assumes at room temperature.

5.9 a) Calculate the dipole energy of a spin 1/2 particle in the field of another spin 1/2 particle 2 Angstroms away. Assuming they are free to rotate, what relative alignment will they assume?

b) Calculate the coulomb energy of two point electrons 2 Angstroms apart.

c) Estimate the magnitude of the Coulomb integral

$$C_{ij} = + \int \psi_a^*(1)\psi_b(2)\frac{e^2}{4\pi\varepsilon_o r_{ij}}\psi_a^*(1)\psi_b(2)\,d\tau$$

$$= + \int \frac{\psi_a(1)\psi_b(2)}{4\pi\varepsilon_o r_{ij}}\,d\tau$$

and the Exchange integral

$$J_{ij} = \pm \int \psi_a^*(1)\psi_b(2)\frac{e^2}{4\pi\varepsilon_o r_{ij}}\psi_a^*(2)\psi_b(1)\,d\tau$$

Compare these with the magnitude of the dipole interaction energy in a) and the electrostatic energy in b).

5.10. Ferromagnetic metals.

a) Explain why ferromagnetism is observed in nickel and not in aluminum.

b) Explain why ferromagnetism is observed in the second half of the 3*d* transition series and not in the first half.