HW 4 solutions:

Problem 4.7

Effective mass in the nearest neighbor tight binding approximation is

$$m^*(k) = \frac{2\hbar^2}{E_b L^2 \cos(kL)}$$

where E_b is the energy band width. In three dimensions $E_b = 12 \times t$ where t is the tight binding hopping integral. GaAs has lattice constant $L = 0.565$ nm and effective electron mass $m^* = 0.07 \times m_0$ near $k = 0$. Hence,

$$t = \frac{2\hbar^2}{L^2 \times 0.07 \times m_0 \times 12} = \frac{(1.05 \times 10^{-34})^2}{(0.565 \times 10^{-9})^2 \times 0.07 \times 9.1 \times 10^{-31} \times 6} = 9.04 \times 10^{-20}\ \text{J}$$

which is

$t = 0.565$ eV.

Problem 4.8

In the nearest neighbor tight binding model energy band width in three dimensions is $E_b = 12 \times t$ where t is the tight binding hopping integral. Since one expects the hopping integral to decrease with increasing lattice spacing, the energy bandwidth should also decrease.

Problem 4.9

A crystal with identical atoms at lattice sites $x_n = nL$, where n is an integer and L is the nearest neighbor atom spacing, has wave function $\psi_{k_x}(x)$ that can be expressed as a direct lattice sum of Wannier functions $\phi(x)$ localized around each lattice site x_n. For identical atoms $\phi(x - x_n) = \phi(x - x_n + nL)$. To show that wave functions of the form

$$\psi_{k_x}(x) = \sum_n e^{ik_x x_n}\phi(x - x_n) = \sum_n e^{ik_x nL}\phi(x - nL)$$

satisfy the Bloch condition we substitute $x = x + L$ to obtain

$$\psi_{k_x}(x + L) = \sum_n e^{ik_x nL}\phi(x + L - nL) = \sum_n e^{ik_x nL}\phi(x - (n-1)L)$$

Let $(n - 1) = m$ so that $n = m + 1$ and $x_m = mL$. Hence,

$$\psi_{k_x}(x + L) = \sum_m e^{ik_x(m+1)L}\phi(x - mL) = \sum_m e^{ik_x mL}\phi(x - mL)e^{ik_x L} = \sum_m e^{ik_x x_m}\phi(x - x_m)e^{ik_x L}$$

Substituting in our expression

$$\psi_{k_x}(x) = \sum_m e^{ik_x x_m}\phi(x - x_m)$$

we get

$$\psi_{k_x}(x + L) = \psi_{k_x}(x)e^{ik_x L}$$

which is the Bloch condition.