ECE215A/Materials206A Fundamentals of Solids for Electronics E.R. Brown/Winter 2008

Quiz#1 Solution Key

1. (a). Defining $U_1 = -\Delta U/2$ and $U_2 = \Delta U/2$, we get

$$f(U_1)=\frac{\exp(-U_1/k_BT)}{\exp(-U_1/k_BT)+\exp(-U_2/k_BT)}=\frac{\exp(\Delta U/2k_BT)}{\exp(\Delta U/2k_BT)+\exp(-\Delta U/2k_BT)}$$

And
$$f(U_2)=\frac{\exp(-U_2/k_BT)}{\exp(-U_1/k_BT)+\exp(-U_2/k_BT)}=\frac{\exp(-\Delta U/2k_BT)}{\exp(\Delta U/2k_BT)+\exp(-\Delta U/2k_BT)}$$

Relative probability is $f(U_2)/f(U_1) = \exp(-\Delta U/k_BT)$, which $\to 0$ as $T \to 0$, and $\to 1$ as $T\to \infty$

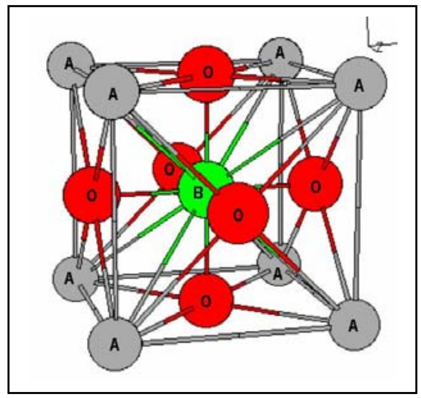
(b) $$\langle U\rangle=\frac{U_1\exp(-U_1/k_BT)+U_2\exp(-U_2/k_BT)}{\exp(-U_1/k_BT)+\exp(-U_2/k_BT)}=\frac{(-\Delta U/2)\exp(\Delta U/2k_BT)+(\Delta U/2)\exp(-\Delta U/2k_BT)}{\exp(\Delta U/2k_BT)+\exp(-\Delta U/2k_BT)}$$

$= -(\Delta U/2)\tanh(\Delta U/2k_BT)$ $\quad \langle U\rangle_{tot} = N\langle U\rangle = = -N(\Delta U/2)\tanh(\Delta U/2k_BT)$

(c) $C_V = d\langle U\rangle tot/dT = N(\Delta U)^2/(4k_BT^2)\,\mathrm{sech}^2(\Delta U/2k_BT) = N(\Delta U)^2/(4k_BT^2)\cosh^{-2}(\Delta U/2k_BT)$. Knowing that $\cosh(0) = 1$, we see that $C_V \to 0$ as $T \to \infty$. And for very small T, $C_V \propto (T)^{-2}\exp(-\Delta U/k_BT) \to 0$.

2. (a) There are two types of elastic waves in every solid, compressional and shear. For compressional, Δr is parallel to k. For shear, Δr is perpendicular to k. The compressional always has higher velocity.

(b) Along the x, y, or z axes, the compressional velocity is defined by $v_C = (C_{11}/\rho)^{1/2}$, and shear velocity is $v_S = (C_{44}/\rho)^{1/2}$, where ρ is the density. Solving each, we find $C_{11} = 1.07\times10^8$ N/m^2 and $C_{44} = 2.81\times10^7$ N/m^2 .



(c) Poisson ratio $\sigma = -\eta_{yy} / \eta_{xx}$, or $-\eta_{zz}/\eta_{xx}$, where η_{xx}, η_{yy}, and η_{zz} are the first three components of the strain vector in any solid. The maximum possible value of σ is +0.5. From clue sheet, the third coefficient $C_{12} \equiv \sigma C_{11}/(1 - \sigma)$, so that $\sigma = 0.36 \Rightarrow C_{12} = 6.07\times10^7$ N/m^2.

3. (a) There are three: (1) simple cubic, (2) body centered cubic, and (3) face-centered cubic.

(b) A little thought (along with the clue) leads to the conclusion that the "underlying" Bravais lattice is simple cubic with one of the A atoms as the reference, the three nearest O atoms as satellite atoms, and the B atom as the other satellite. In other words, it is a five-atom basis: one A, one B, and three Os. This basis, when translated through space by the simple-cubic lattice vectors produces the entire Perovskite structure with no extra or missing atoms.

(c) When all the atoms in the Perovskite structure are the same, the underying Bravais lattice that has the smallest possible cubic primitive cell is the face-centered cubic with the center atom as the one satellite. But a little thought shows that the crystal does not "look the same" from each fcc atom (e.g., looking half-way along the body diagonal from a corner atom leads to the cube-centered atom, but looking along the same direction from a face atom does not reveal any atom). So we deduce that the cubic Perovskite structure with all the atoms identical leads to a simple cubic structure with a five-atom basis (note: this is not so unusual, since replacing the two different atoms in a zincblende structure, such as GaAs, does not yield a Bravais lattice either…. rather it results in the diamond crystal).

4(a). There are three lattice wave solutions, one longitudinal acoustic (LA) and two transverse acoustic (TA). The LA corresponds to the compression wave of elastic theory, and the two TAs correspond to the two shear waves of elastic theory?

(b). Under this wavelength condition, the circular frequency reaches a maximum, and $k = \pi/d$. The group velocity $d\omega/dk = 0$ under this condition. The value $k = \pi/d$ corresponds to the Nyquist sampling frequency in discrete-time sampling (i.e., digital signal processing).

c) Yes, there are optical lattice-wave solutions, one longitudinal optical (LO) wave and two transverse optical (TO) for each additional atom in the basis beyond the first. So for the given crystal, we expect three additional LO lattice waves, and six additional TO lattice waves, or nine total optical lattice waves.

d) There will still be one LA and two TA waves, and just one LO wave and two TO waves.