Midterm Examination for
Introduction to Nanotechnology (I)

Name: ________________________ November 11, 2005

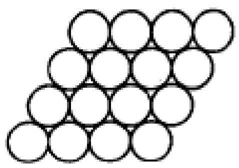
Q1. (A) Consider the periodic two-dimensional solid with part of it as shown in Fig 1A. The white atoms form a closed pack hexagonal structure.

(a) Indicate the unit cell and lattice vectors. (3%)

(b) Let the radius of the white atoms be a_0. What is the size (area) of a unit cell in terms of a_0? (4%)

(c) How many white atoms are there per unit cell? (3%)

Fig 1A:



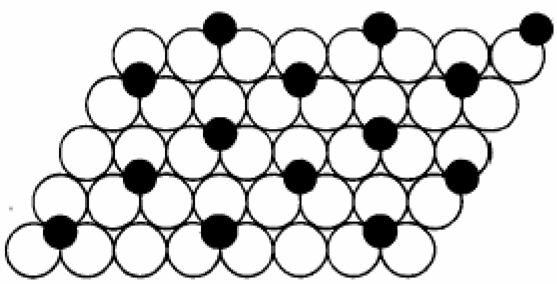
(B) Consider now the periodic two-dimensional solid with part of it as shown in Fig 1B. The white atoms form a closed pack hexagonal structure, and each black atom sits on top of three white ones.

(a) Indicate the unit cell and lattice vectors. (3%)

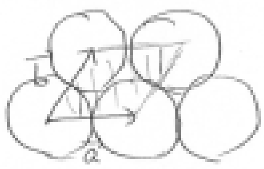
(b) Let the radius of the white atoms be a_0. What is the size (area) of a unit cell in terms of a_0? (4%)

(c) How many white atoms are there per unit cell? (3%)

Fig 1B:

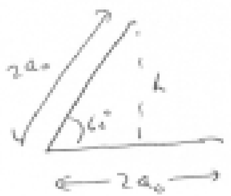


Q1A. (a) There are many choices possible for the unit cell and lattice vectors, one possible choice is



[translation of unit cell by lattice vectors $\vec{a}$ and $\vec{b}$ alone must cover entire lattice]

(b)

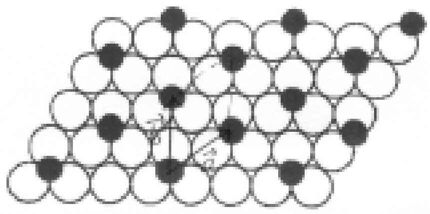


$$h = 2a_0 \cdot \sin(60^\circ) = 2a_0 \cdot \frac{\sqrt{3}}{2} = \sqrt{3}\, a_0$$

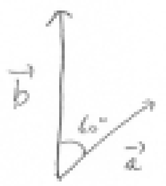
$$\text{area} = 2a_0 \cdot \sqrt{3}\, a_0 = 2\sqrt{3}\, a_0^2$$

(c) one atom per unit cell

B (a) One possible choice is :



(b)



Comparing with part A, can see that

length of $b = 2h = 2\sqrt{3}\,a_0$ = length of a

$$\text{area} = (2\sqrt{3}\,a_0)^2 \sin 60^\circ = 4\cdot 3\, a_0^2 \cdot \frac{\sqrt{3}}{2}$$

$$= 6\sqrt{3}\, a_0^2$$

(c) either by counting, or take the ratio between unit cell area here and that of part A

$$\text{number} = \frac{6\sqrt{3}\,a_0^2}{2\sqrt{3}\,a_0^2} = 3 \quad \text{white atoms per unit cell}$$

Q2. A one-dimensional solid, with one atom per unit cell and lattice size a, is well described by a tight-binding Hamiltonian such that the energy dispersion is given by the relation

$$E(k) = -2t\cos(ka)$$

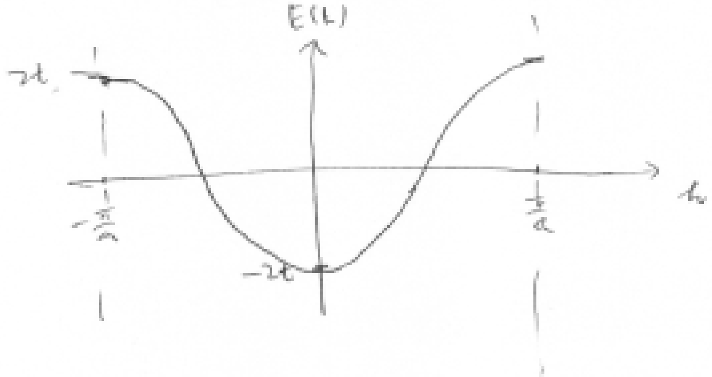
(a) Sketch this relation. (5%)

(b) Calculate and sketch the density of states. (7%)

(c) Suppose the electron density per unit length is given by 1/(2a) (that is, one electron every two atoms). Calculate the Fermi energy in terms of t. (8%)

Q2. $E = -2t\cos(ka)$

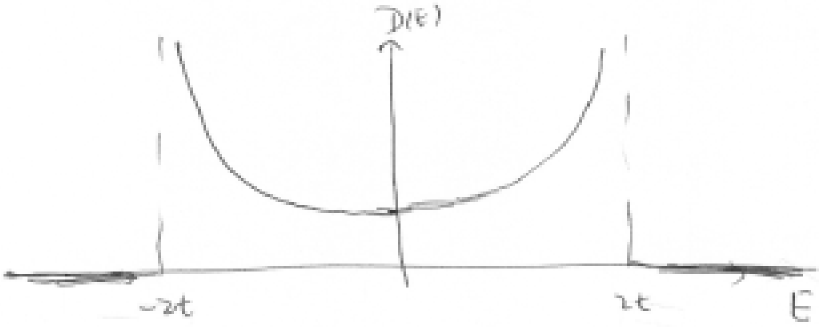
(a) sufficient to sketch $E(k)$ for $-\frac{\pi}{a} < k < \frac{\pi}{a}$



(b) density of states (per spin) per unit length

$$D(E) = \frac{dk}{2\pi\, dE} = \frac{1}{2\pi\left(\frac{dE}{dk}\right)}$$

$$= \frac{1}{(2\pi)(2ta)(\sin ka)} \overset{|E|<2t}{=} \frac{1}{(2\pi)(a)}\frac{1}{\sqrt{(2t)^2 - E^2}}$$



[$D(E) = 0$ for $|E| > 2t$]

(c) Density of electrons per unit length $= \frac{1}{2a}$

per spin: $\frac{1}{4a}$

energy lowest near $k = 0$, so

occupied from $-k_{max}$ to k_{max} so that

$$\frac{2k_{max}}{2\pi} = \frac{1}{4a}$$

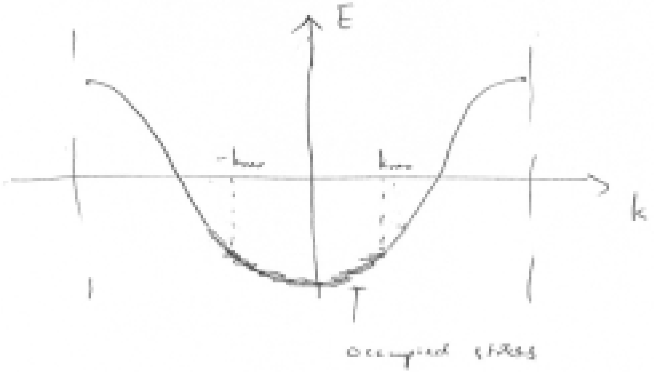
$$k_{max} = \frac{\pi}{4a}$$

Fermi energy $= E(k_{max})$

$$= -2t\cos(k_{max}\,a)$$

$$= -2t \cdot \cos\left(\frac{\pi}{4}\right) = -\sqrt{2}\,t$$

[A sketch is always helpful:



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Q3. (a) List the three types of information obtainable on a modern AEM. (5%)

(b) List at least five signals that are produced due to the interaction of high energy electrons with the thin specimen in TEM. (5%)

Answer: (a) Image, structure, and chemistry (ref. course note, p-27)

(b)Transmitted electrons, elastically scattered electrons (diffracted electrons, for crystalline material), inelastically scattered electrons, back scattered electrons, secondary electrons, X-rays (characteristic and Bremsstrahlung), photons (for some semiconductors, minerals, and ceramics), phonons, heat…………(ref. course note, p-05)

Q4. An SAD pattern of polycrystalline Au standard specimen is shown below. This SAD pattern was taken on a TEM operated at 200 kV such that the electron wavelength should be 0.002508 nm. Measure approximately the ring diameters in this pattern and then calculate the camera length used. (10%)

(Hint: For cubic crystals,

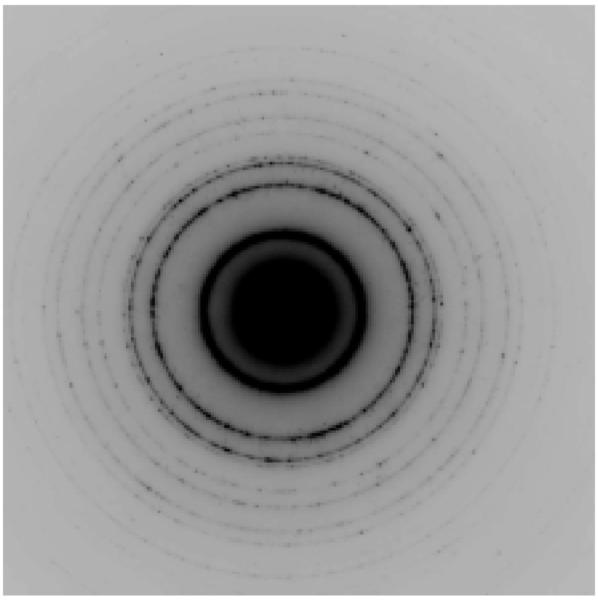
$$d_{hkl} = a_o / (h^2 + k^2 + l^2)^{1/2}$$

R1 : R2 : R3 : ……. = 1 : 1.155 : 1.633 : 1.915 : 2.000 (for FCC metal)

= 1 : 1.414 : 1.742 : 2.000 : 2.236 (for BCC metal).

Rd = λL; meanwhile the d-spacings of gold are also given below in the unit of angstroms.)

d(A)	h	k	l
2.3553	1	1	1
2.0398	2	0	0
1.4423	2	2	0
1.2300	3	1	1
1.1776	2	2	2



Answer: Measuring approximately the ring diameters in this pattern, you will get Rp, Rq, Rr, and Rs. Since ring p is broadened, it is quite possible that it is the result of two or more overlapping rings.

Comparing the values of Rq, Rr, and Rs you have measured, you will find out that:
Rq : Rr : Rs : 1.6 : 1.9 : 2.0, very close to 1.633 : 1.915 : 2.000.
It is now clear that you are working on an FCC system (surely, Au is an FCC metal, don't you know?).

Since for cubic crystals, $d_{hkl} = a_o / (h^2 + k^2 + l^2)^{1/2}$, and
R1 : R2 : R3 : ….= 1 **:** 1.155 **:** 1.633 **:** 1.915 **:** 2.000 (FCC metal), we deduce that:

$R_{\{111\}} : R_{\{200\}} : R_{\{220\}} : R_{\{311\}} : R_{\{222\}} = 1/d_{111} : 1/d_{200} : 1/d_{220} : 1/d_{311} : 1/d_{222}$

$= \sqrt{3} : \sqrt{4} : \sqrt{8} : \sqrt{11} : \sqrt{12}$

$= 1 : 1.155 : 1.633 : 1.915 : 2.000$

Thus we now know **$R_{\{220\}}$= Rq, $R_{\{311\}}$= Rr, and $R_{\{222\}}$= Rs.**
Choose one of the three rings, say $R_{\{311\}}$= Rr, you can easily calculate the camera length L by using the formula Rd = λ L.
(ref. course note, p-34)

Q5. Please describe how the scanning tunneling microscopy works and explain why scanning tunneling microscopy can achieve atomic resolution on the surface of conducting materials. (10%)

Answer: The scanning tunneling microscopy operates based on the quantum phenomenon of tunneling. When two conductive objects (tip and sample) are brought within about 1nm and a suitable bias voltage is applied, a tunneling current will flow. By controlling this current with a feedback circuitry during the two-dimensional scan of the tip, the surface topography of the sample can be imaged.

In the tunneling regime, if the distance between the tip and the surface decreases by 1 Å, the tunneling increases by about one order of magnitude. Therefore, if an atom sticks out by 1 Å (or more) than other tip atoms, the major contribution of the tunneling would come from that outmost atom. The surface atom directly underneath that tip atom would be imaged. That is why STM can achieve atomic resolution easily.

Q6. Please describe the differences in operation among the three common imaging modes, ie. contact, non-contact, and intermittent contact, of the atomic force microscopy, and the advantage and disadvantage of these modes. (10%)

Answer: 1. Contact mode: the probe is pushed against the sample surface in the repulsive force range.
Advantage: high imaging resolution can be achieved.
Disadvantage: the sample and probe are easily damaged.

2. Non-contact mode: the probe is brought toward the sample surface in the attractive force range and the imaging is performed with the probe vibrating with small amplitude.
   Advantage: the interaction between the sample and probe is reduced and they can sustain for a longer lifetime of imaging.
   Disadvantage: high resolution images are more difficult to obtain.
3. Intermittent contact mode: the probe vibrates with large amplitude so that it will make an intermittent contact with the sample.
   Advantage: the probe is kept away from the sample for most of time, so the conditions of the probe and sample can be preserved longer meanwhile the high imaging resolution can be achieved.

Q7. Calculate the energy separation near the Fermi surface of a metallic cluster of 10 nm in diameter, which is comprised from a divalent metal element of 0.25 nm in dia. Assume the Fermi energy is 8 eV for the bulk material of the same metal. (10 %)

Answer: The total number of atoms in the cluster is $(10\ nm/0.25\ nm)^3 = 64000$ and the number of electrons in the cluster is 2 x 64000 = 128,000. Since each state can accommodate two electrons, the number of states is 64000. In addition, the Fermi energy is only related to the electron density, i.e., independent of the size. Therefore, the energy separation is 8 eV/64000 = 0.125 meV.

Q8. Magic numbers often exhibit in small clusters. According to your knowledge, (a) write down a few magic numbers for noble gas clusters and alkali metal clusters, separately. (5%) (b) What are the origins of these numbers, respectively? (5%)

Answer: (a) For noble gas clusters: 13, 19, 25, 55, 147…
For alkali metal clusters: 2, 8, 18, 20, 34, 40, 58…
(b) For noble gas clusters: the major factor is due to the stability associated with a closed-shell geometric structure.
For alkali metal clusters: the major factor is due to the stability associated with a closed-shell electronic structure.