Solutions for 2005 Final Exam
Introduction to Nanotechnology- An Overview I

1 (10 points) Below is the plot showing the mass spectrum of Pb clusters. Please explain the term of "Magic number of atoms" in nanoparticle and cluster What is it and its mechanism?

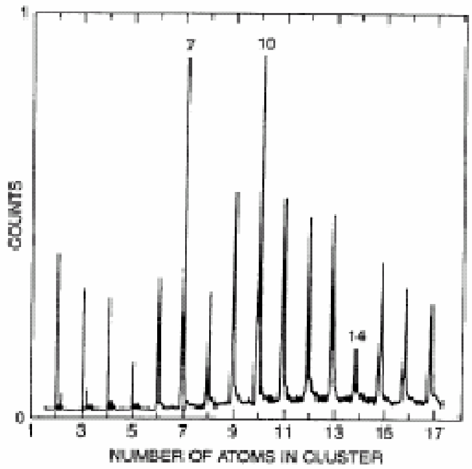


Figure 4.3. Mass spectrum of Pb clusters. [Adapted from M. A. Duncan and D. H. Rou
Am. 110 (Dec. 1989).]

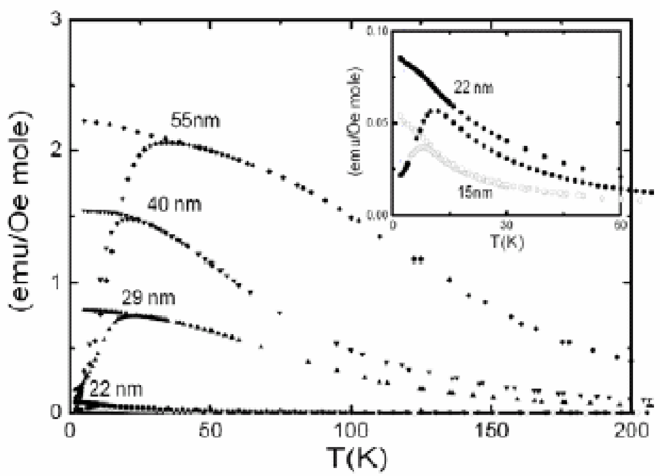
2. (10 points) Below is the plot of χ vs. T for $FeSi_2$ nanoparticles. Please explain

a. The term of "Paramagnetism"

b. What is the Blocking temperature?

c. the reason for the difference. of FC and ZFC curves,

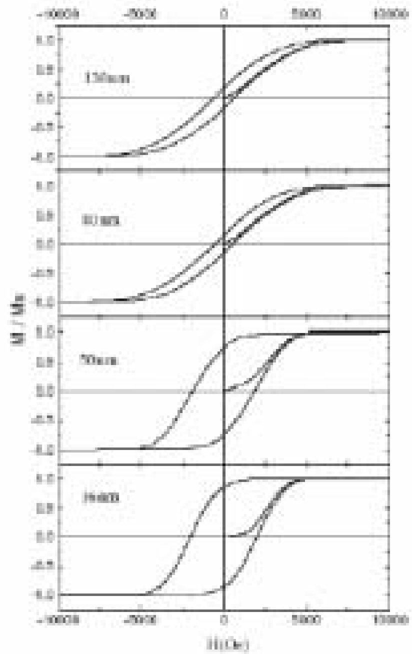
d. Why T_B is proportional to K and V ? please explain it.

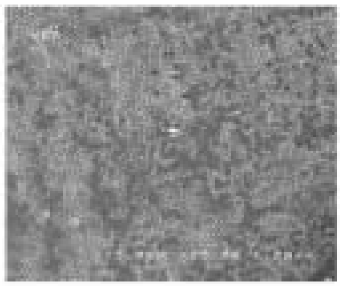


$$T_B = \frac{KV}{25k_B}$$

3. (10 points) Please explain "Phonon quanum size effect" and "Electronic quantum size effect"

4. (10 points) The following plot is the magnetization vs. magnetic field for Fe nanowires in AO template (as below). Would you please explain why does the hysteresis loop become bigger as diameter decreases？



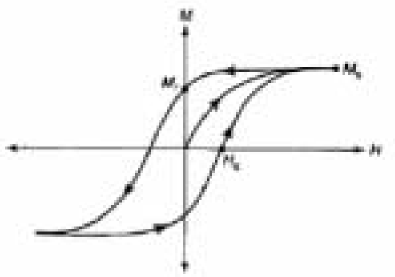


5. (10 points)

a. Please explain "coercive field", "remnant magnetization" and "saturation magnetization"

b. Please explain the plot of remanent magnetization vs diameter and explain its mechanism.

c. Hard magnet? Soft magnet?



7.3. Plot of the magnetization M versus an applied magnetic field H for a hard ...gnetic material, showing the hysteresis loop with the coercive field H_c, the remnant ...ization M_r, and the saturation magnetization M_s, as indicated.

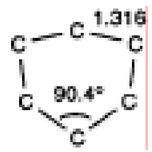
6. (10 points bonus) Please describe the diameter (size) effect on the mechanical properties for bulk nanostructured materials. elastic or inelastic ? Hardening, ductile or brittle?

7. **(a)** (5 points) Calculations of the structure of small carbon clusters by molecular orbital theory show the clusters form two types of geometries depending on the number of atoms *N* in the clusters. Please make schematic drawings to illustrate the geometries for *N* = 6, 7, 8 and 9.
(b) (5 points) What is the diameter of C60 fullerenes? Is pure C60 an electrical insulator or a superconductor? What is the smallest fullerene that has been synthesized?

Solution:

(a)

N=6



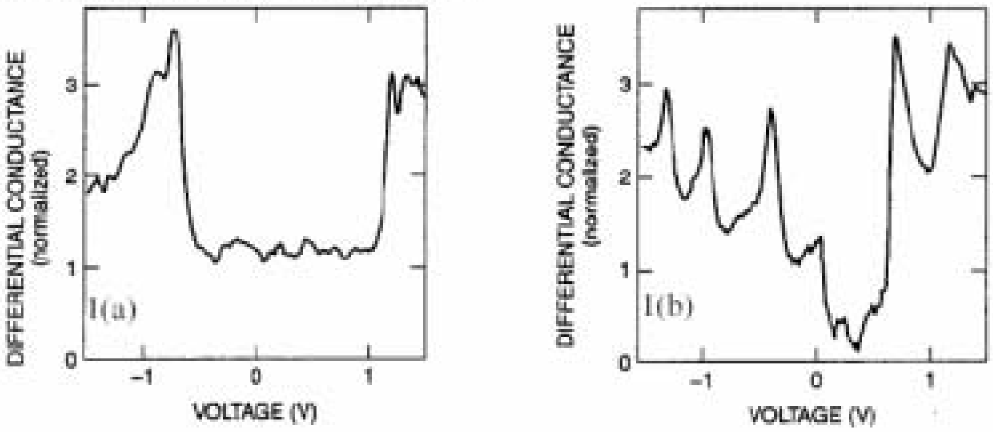
N=7

N=8

N=9

(b) Diameter of C60 fullerenes = 0.71nm. Pure C60 is an insulator
Smallest fullerene = C20.

8. **(a)** (5 points) The measured (dI/dV)/(I/V) curves for two single-walled carbon nanotubes with chiralities (11,7) and (9,9) are displayed below. What are the tube chiralities for these curves? Why you choose so. [Reference: Cees Dekker (Physics Today, May, 1999, pp.22-28)]



(b) (5 pints) The following 4 curves are dI/dV curves measured for four semiconductor single-walled carbon nanotubes with different diameters: one 1.2nm, two 1.4nm and one 2.0nm. What are the corresponding tube diameters for these curves? Why you choose so? [Reference: Wildoer et al. Nature, 391, 59 (98)]

Solution:

(a) 1(a) (9,9); 1(b) (11,7);

n=m → Armchair → always metallic

11-7 = 4 (not a integer multiple of 3) → semiconductor

(b) 2(a) 1.2nm; 2(b) 2.0nm; 2(c) 1.4nm; 2(d) 1.4nm

The wilder the tube the smaller the semiconductor gap.

9. **(a)** (5points + 3-point bonus) The sizes of unit cell in *k*-space for two and three spatial dimensions with area L^2 and volume L^3 are $(2\pi/L)^2$ and $(2\pi/L)^3$, respectively. Assuming an effective electron mass of m^*, please drive the density of states as a function of energy E for two dimensions D_{2D} and for three dimensions $D_{3D}(E)$.

(b) (5 point + 5-point bonus) For a two dimensional film with thickness L_Z, the confinement along *z*-axis results in quantized k_Z values in unit of $2\pi/L_Z$ and quantized energy in unit of $\varepsilon_Z = \hbar^2\pi^2/2m^* L_Z^2$. The 2D density of states for this confined system forms subbands:

$$D_{2D\,confined}(E) = D_{2D}\sum_p \vartheta(E - p^2\varepsilon_Z),$$

where $\vartheta(x) = 1$ if $x \ge 0$ and $=0$ if $x<0$, and p is the subband index.

For thick films (large L_Z), ε_Z is small, and $D_{2Dconfined}(E)$ approaches $D_{3D}(E)$. Please compare the confined 2D density of states with the 3D density of states by plotting them as a function of energy in the same graph, and equate the values at the crossing points for p=1, 2 and 3 by setting the volume in $D_{3D}(E)$ as L^2L_Z. The vertical axis is density of states in unit of D_{2D} (which is the 2D density of states in the first subband and is a constant), and the horizontal axis is energy E in unit of ε_Z. If you are not able to make a quantitative comparison, please at least make a schematic drawing.

Solution:

(a) For 2D, Fermi region=πk_F^2,

$$N_{2D}(E) = \frac{2\cdot\pi k_F^2}{(2\pi/L)^2} = \frac{L^2}{2\pi}\left(\frac{2m^*}{\hbar^2}\right)E,\quad D_{2D} = \frac{dN(E)}{dE} = \frac{L^2}{2\pi}\left(\frac{2m^*}{\hbar^2}\right)$$

For 3D, Fermi region=$\frac{4\pi}{3}k_F^3$,

$$N_{3D}(E) = \frac{2\cdot(4\pi k_F^3/3)}{(2\pi/L)^3} = \frac{L^3}{3\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}E^{3/2},\quad D_{3D}(E) = \frac{dN(E)}{dE} = \frac{L^3}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}E^{1/2}$$

(b) $D_{2D\,confined}(E) = D_{2D}\sum_p \vartheta(E - p^2\varepsilon_Z),\quad \varepsilon_Z = \hbar^2\pi^2/2m^*L_Z^2$

for p=1, $E=\varepsilon_Z$

$$D_{2Dconfined}(\varepsilon_Z) = D_{3D}(\varepsilon_Z) = \frac{L^2 L_Z}{2\pi^2}\left(\frac{2m^*}{\eta^2}\right)^{3/2} \varepsilon_Z^{3/2} = \frac{L^2 L_Z}{2\pi^2}\left(\frac{2m^*}{\eta^2}\right)^{3/2}\left(\frac{\eta^2\pi^2}{2m^* L_Z^2}\right)^{1/2} = \frac{L^2}{2\pi}\left(\frac{2m^*}{\eta^2}\right) = D_{2D}$$

for p=2, $E=4\varepsilon_Z$

$$D_{2Dconfined}(4\varepsilon_Z) = D_{3D}(4\varepsilon_Z) = \frac{L^2 L_Z}{2\pi^2}\left(\frac{2m^*}{\eta^2}\right)^{3/2} 2\varepsilon_Z^{1/2} = 2\frac{L^2 L_Z}{2\pi^2}\left(\frac{2m^*}{\eta^2}\right)^{3/2}\left(\frac{\eta^2\pi^2}{2m^* L_Z^2}\right)^{1/2} = 2\frac{L^2}{2\pi}\left(\frac{2m^*}{\eta^2}\right) = 2D_{2D}$$

for p=3, $E=9\varepsilon_Z$

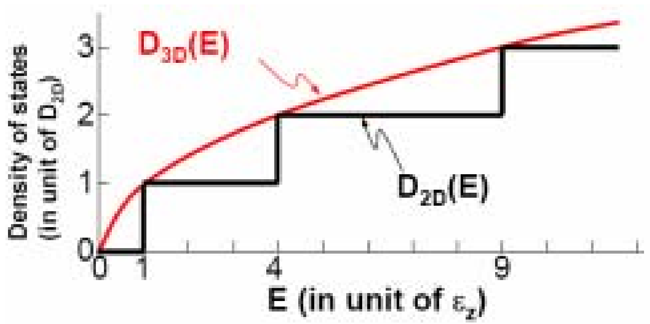
$$D_{2Dconfined}(9\varepsilon_Z) = D_{3D}(4\varepsilon_Z) = \frac{L^2 L_Z}{2\pi^2}\left(\frac{2m^*}{\eta^2}\right)^{3/2} 3\varepsilon_Z^{1/2} = 3\frac{L^2 L_Z}{2\pi^2}\left(\frac{2m^*}{\eta^2}\right)^{3/2}\left(\frac{\eta^2\pi^2}{2m^* L_Z^2}\right)^{1/2} = 3\frac{L^2}{2\pi}\left(\frac{2m^*}{\eta^2}\right) = 3D_{2D}$$

For $0<E<\varepsilon_Z$, $D_{2D\,confined}(E) = 0$

For ε_Z,$<E<4\varepsilon_Z$, $D_{2D\,confined}(E) = D_{2D}$

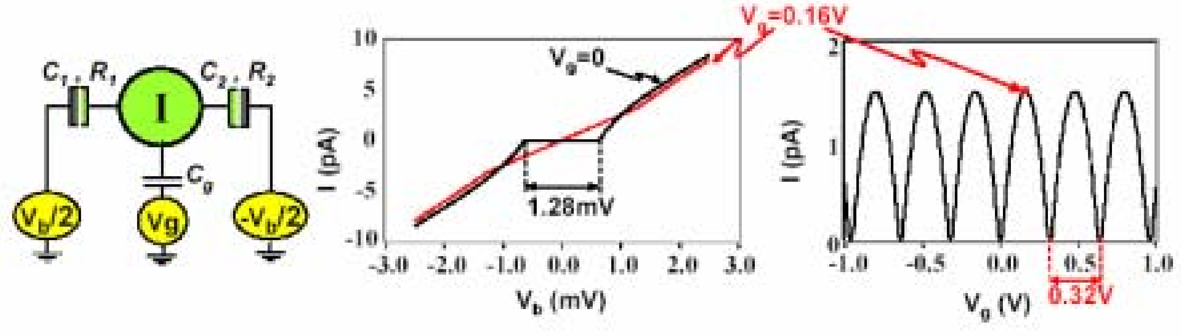
For $4\varepsilon_Z<E<9\varepsilon_Z$, $D_{2D\,confined}(E) = 3D_{2D}$

For $9\varepsilon_Z<E<12\varepsilon_Z$, $D_{2D\,confined}(E) = 4D_{2D}$



10. **(a)** (5 points + 2-point bonus) The figures below show (left) the biasing circuit of a single electron transistor and (middle) the calculated current-bias voltage (IV_b) characteristics at $V_g = 0$ and $V_g = 0.16$V and (right) current-gate voltage (IV_g) characteristic at V_b=0.6mV. The curves are calculated for T=50mK, which corresponds to thermal energy much smaller than the charging energy of the device. At V_g=0, the device displays a sharp Coulomb blockade feature with threshold voltage V_{th}=1.28mV/2=0.64mV. The blockade feature can be lifted by the gate field, and the current reaches the maximum values at V_g=0.16. When ramping gate voltage, the current shows periodic modulation with a period ΔV_g=0.32V. From these curves, please figure out the sum capacitance C_Σ seen by the island (*i.e.* $C_\Sigma = C_1+C_2+C_g$), and the gate capacitance value C_g. (note: e=1.6×10^{-19} Coulomb)

(b) (5 points) The above calculation assumes the tunnel junction resistance R_1=R_2=100MΩ. If the resistance value is too low, the Coulomb blockade feature will be smeared. Please give an order of estimate for the required minimum resistance value, and state the reason.



Solution:

(a) $2E_C$=0.64meV, e/C_Σ=0.64mV, C_Σ=e/0.64mV=1.6×10^{-19}C/6.4×10^{-4}V= 250×10^{-18}F

(b) e/Cg=0.32V, Cg=e/0.32V=1.6×10^{-19}C/0.32V=0.5aF

11. **(a)** (5 points) Drive the mean level spacing of metal particles using the formulae obtained from Problem 9(**a**). Calculate this value (in unit of eV) for an Au-spherical particle with diameter 5nm. (note: k_F for Au = 12.1nm^{-1};

$$\frac{6}{\pi}\frac{\hbar^2}{me} = 5.75\times10^{-18}\left[\frac{\mathrm{J}^2\cdot\mathrm{s}^2}{\mathrm{kg}\cdot\mathrm{C}}\right]$$

; If you are not able to solve Problem 9, please then write down the formula for the discrete energy levels)

(b) (5 points) The discrete energy levels may be smeared by thermal fluctuations as well as fast electron relaxation process. Please estimate criteria in terms of temperature and in terms of electron relaxation time for appreciation of the discrete levels in a 5nm-diameter Au particle. (note: Planck's constant $\hbar/2\pi = 1.055\times10^{-34}$ Js, Boltzmann constant $k_B = 1.38\times10^{-23}$J/K, $1eV = 1.16\times10^4\mathrm{K} = 1.6\times10^{-19}\mathrm{J}$, $e/\hbar = 3.85\times10^{13}$ [$C/J\cdot s$]; If you are not able to solve (**a**), please write down the appropriate formulae that are to be used for the estimations.)

Solution:

(a) $$\delta = \frac{2}{D(\varepsilon_F)} = \frac{2}{\frac{Vol}{2\pi^2}\left(\frac{2m}{\eta^2}\right)^{3/2}E^{1/2}} = \frac{2}{\frac{Vol}{2\pi^2}\left(\frac{2m}{\eta^2}\right)^{3/2}\frac{\eta k_F}{(2m)^{1/2}}} = \frac{4\pi^2}{Vol\,\frac{2m}{\eta^2}k_F} = \frac{2\pi^2\eta^2}{mk_F Vol}$$

in unit of eV, $$\frac{\delta}{e} = \frac{2\pi^2\eta^2}{mek_F Vol} = \frac{h^2}{2mek_F\left(\frac{4}{3\cdot 8}\pi D^3\right)} = \frac{6h^2}{2mek_F\pi D^3} = \frac{1}{2D^3k_F}\frac{6h^2}{\pi me}$$

$$\frac{\delta}{e} = \frac{1}{2D^3k_F}5.75\times10^{-18}\frac{\mathrm{J}^2\cdot\mathrm{s}^2}{\mathrm{kg}\cdot\mathrm{C}} = \frac{5.75\times10^{-18}}{2\cdot125\cdot12.1\times10^{-18}}\frac{\mathrm{J}^2\cdot\mathrm{s}^2}{\mathrm{m}^2\cdot\mathrm{kg}\cdot\mathrm{C}} = 1.9mV \quad \text{or} \quad 21.934\mathrm{K}$$

(b) δ=1.89meV=21.934K $\rightarrow$ T << 21.9K

δ=1.89meV $\rightarrow$

$$t_{relax} >> \frac{\eta}{\delta} = \frac{\eta}{1.9\mathrm{m}e\mathrm{V}} = \frac{\eta}{e}\frac{1}{1.9\times10^{-3}V} = \frac{1}{3.85\times10^{13}\times1.9\times10^{-3}}\frac{\mathrm{J}\cdot\mathrm{s}}{\mathrm{C}\cdot\mathrm{V}} = 0.137\times10^{-10}\mathrm{s} = 1.37\mathrm{ns}$$