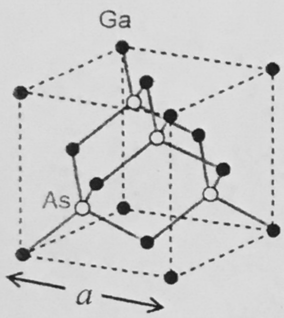
*Any additional details wrong : −1

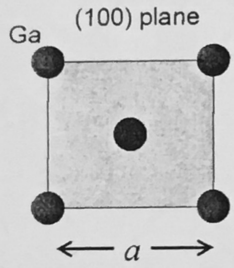


**Your name:** ______________________ **Your Score:** ______________________

1. **Structure and mechanics of crystalline solids (20 points)**

a. The following is the unit cell of GaAs (zincblende structure). On average how many Ga atoms are there and how many As atoms are there per unit cell? What is the coordination number for Ga and As, each? The following also shows the atomic arrangement of a (100) plane on the surface of the shown unit cell. Please draw a similar image of atomic arrangements on a (111) plane of this unit cell, and label which atoms are Ga and which are As, and label the side lengths of this (111) plane, using **a**.



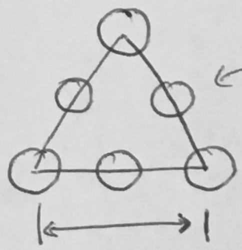




Ga = 4 atoms/unit cell (+2)

As = 4 atoms/unit cell (+2)

CN for Ga : 4 (+1)

'' As = 4 (+1)



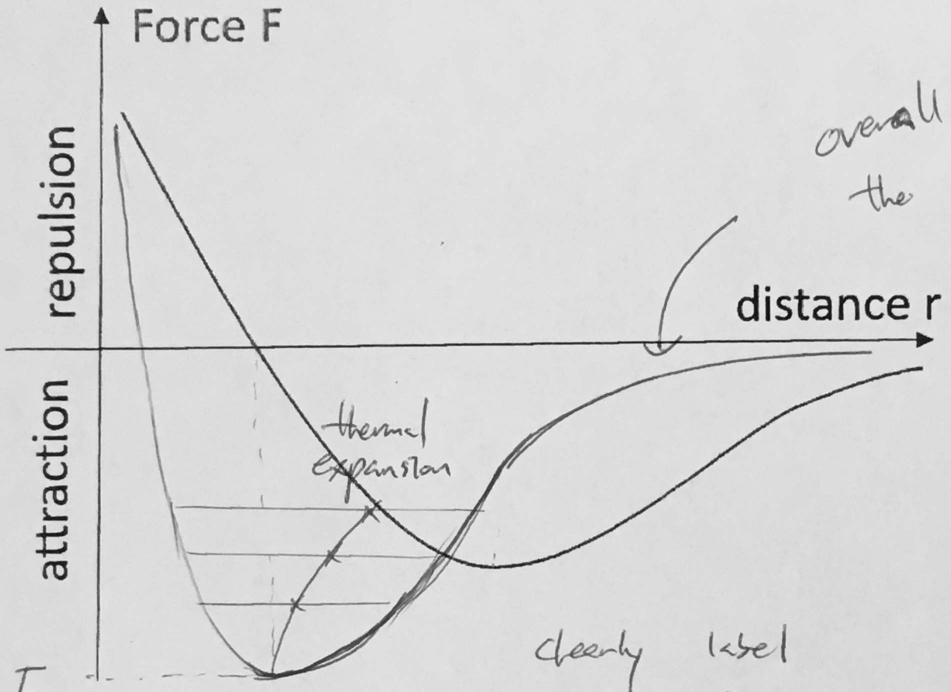
← all Ga atoms

(+4)

$\sqrt{2}a$

Total 10 points

b. The following is the force F between two atoms in a solid. Please draw *schematically*, **in the same figure**, the corresponding potential energy E between them as a function of their distance *r*. Please describe briefly how you ended up with the E vs. r plot based on the force plot given. Label equilibrium distance $r_0$ and bond energy $E_0$ on your plot (pay attention that your E and F should align well along the *r* axis). Based on these plots, explain in a few lines the fact that solids typically have thermal expansion (i.e., increasing temperature causes overall lattice expansion).




overall shape of the plot (+2), the entire curve could be shifted along y-axis (e.g. Ionic bonding) that is $E \to 0$ at $r \to \infty$, not always.

label $E_0$ (+1)

$r_0$ ⇒ clearly label $r_0$ at $F_{attraction} = F_{repulsion}$ (+3)

Describe that $F = -\frac{dE}{dr}$, which is on the first page of the exam (+1)
(you could also explain in words)

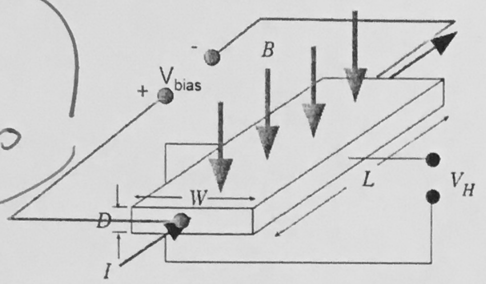
E vs. r curve asymmetric, average distance btw the two end points for same energy increases w/ rise in E (+3) (as long as your explanation is correct)

MSE111, Midterm Exam, Spring 2017, Prof. J. Wu
Closed book, equations are provided

**2. Electrical transport (20 points)**

a. Explain in a few lines the principle of Hall effect. A schematic is shown below. Add more schematics to help your explanation if necessary. What physical quantities can be measured using this method?

total +10




moving electrons (or charge carriers) experience Lorentz force due to magnetic field applied. (+3)

Electric field generated by the separated charge creates force that balances the Lorentz force ~~due~~ due to B. (+3)

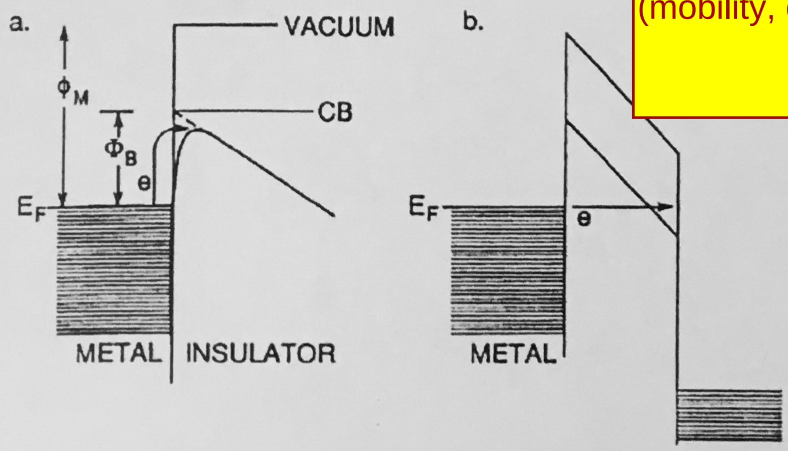
At steady-state, Hall field (or Hall voltage) is measured across the sample. (+2)

Can measure Hall coefficient ($R_H = \pm \frac{1}{en}$) → tells you (+1) sign of charge carriers + concentration. (+1)

~~(+2)~~

b. Below are two possible conduction mechanisms for a thin insulator. Explain in a few sentences each of these two mechanisms; explain how to design experiments to differentiate these two mechanisms.

One should at least mention sign of carriers (+1), and any other quantities (mobility, carrier concentration……, +1)




a. Thermionic (Schottky) emission (thick barrier)
b. Quantum tunneling (thin barrier)

(+4)

Schottky emission : 1) electrons thermally activated to overcome schottky barrier ($\phi_B$) to be injected to a dielectric (CB)

or 2) electrons thermally activated to overcome metal's workfunction ($\phi_m$) to be ejected to vacuum.

(+4)

Quantum tunneling : electron wavefunc extended across the thin insulator (or the barrier), electron tunnels across the barrier.

Reasonable experiment to differentiate the two (+2)

total +10

**3. Thermal transport (10 points)**

The thermal conductivity of a crystalline material has two components, contribution from lattice, $k_{\text{lattice}}$, and contribution from electrons $k_{\text{electronic}}$. Here $k_{\text{lattice}}$ is low at low temperatures, and low at high temperatures, while peaks at some intermediate temperature (tens of K). Explain in details what physics causes the low $k_{\text{lattice}}$ at very low temperatures, and what process causes the low $k_{\text{lattice}}$ at very high temperatures. (Hint, remember the phonon scattering process, and $k_{lattice} = C_v \cdot v \cdot l / 3$, where $C_v$ = specific heat, $v$ = sound velocity, and $l$ = phonon mean free path).

1) at very low T $\Rightarrow$ $C_v \propto T^3$ $\Rightarrow$ low T, low $k_{\text{lattice}}$ (+3)

phonon density low, phonon-phonon scattering insignificant (+2)

$l$ not limiting

2) at high T $\Rightarrow$ $C_v$ is constant (3R) (+2)

phonon density $\propto$ T, high density $\rightarrow$ phonon-phonon scattering increase.

$l$ (phonon mean free path) $\propto \frac{1}{T}$ (+3)

therefore, low $k_{\text{lattice}}$.

total 10 points

**4. Quantum physics (30 points)**

a. Using Heisenberg's uncertainty principle, estimate (i.e., find an approximate expression without solving the Schordinger equation) the ground state energy of an electron confined in an infinitely deep, 1D square well with well width $L$. Show details.

Heisenbergs uncertainty $\Delta p \cdot \Delta x \approx h$ (+1)  total 6points

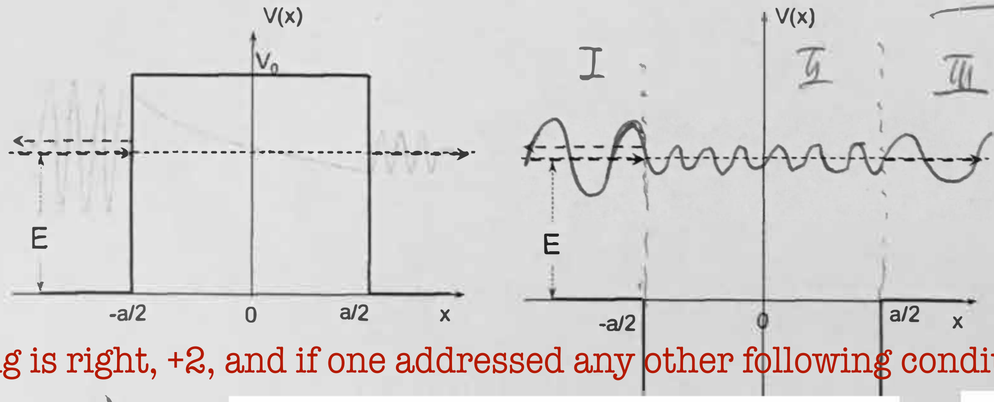
$\Delta x = L$  $\Delta p = h/L$ (+2)

① electron in an infinitely deep well propagates in $+x$ and $-x$ directions
→ momentum also positive & negative
$p = h/2L$ (+1) $E = \frac{p^2}{2m} = \frac{h^2}{8mL^2}$ (+2)

② assume $p$ at least of the order of $\Delta p$
$p \approx h/L$ (+1)
$E = \frac{p^2}{2m} = \frac{h^2}{2mL^2}$ (+2)

b. On the left hand side the wavefunction of a tunneling electron is schematically shown. If the barrier becomes a well with a depth $V_0$ (note that here $V_0$ itself is a positive number), then the situation is different. Please draw similarly the electron wavefunction in the three regions for this case. Please pay attention to wavefunctions connections, their relative amplitude, and their relative period (or wavelength). Clearly indicate how the amplitude and the wavelength differ in all three regions, or whether it should not be different. (Here, consider the case where tunneling probability (T) or the probability of transmission is less than one. Resonant tunneling (T=1) will be discussed in the next question)

total 12points




If the drawing is right, +2, and if one addressed any other following condition, +2/each

① $\lambda_{II} < \lambda_{I}$

② $\lambda_{III} = \lambda_{I}$

③ amplitude in III < amplitude in I (since $T<1$) )

④ amplitude II < amplitude I, III (same here)

⑤ if $\psi$ or $\frac{d\psi}{dx}$ ~~not~~ continuous )

2 way of solving it, but the grading would only follow one which gives you more points (than the other)

total +12



c. The tunneling probability T for the left-hand-side case is given in the equation sheet. Please derive the new expression of T for the right-hand-side case, and prove that when $n\lambda=2a$ ($\lambda$ is electron wavelength in the well region, n=1, 2, 3,…), T becomes 100% (resonant tunneling). What are the values of E for these resonant tunneling events? (Please make sure your T expression contains only real parameters, no imaginary parameters, and clearly define your parameters in the expression!)

Start from T (for left-hand side) $= \dfrac{1}{1+D(\sinh \alpha a)^2}$ (+1)

$$D = \frac{V_0^2}{4E(V_0-E)} \quad (+1)$$

T and D for region II, where

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E-V_0)\psi = 0 \qquad \psi_{II} = B_1\exp(\alpha x) + B_2\exp(-\alpha x)$$

$$\alpha = ik, \quad k = \frac{\sqrt{2m(E-V_0)}}{\hbar}$$

Now for RHS case, $E+V_0$ ($E-V$, $V=-V_0$)

Then $D = \dfrac{V_0^2}{4E(-V_0-E)}$, $T = \dfrac{1}{1+D\{\sinh(ika)\}^2}$, $k = \dfrac{\sqrt{2m(E+V_0)}}{\hbar}$ (+2)

$$T = \frac{1}{1+\dfrac{V_0^2}{4E(-V_0-E)}\{\sinh(ika)\}^2} = \frac{1}{1+\dfrac{V_0^2}{4E(E+V_0)}\left\{\dfrac{\sinh(ika)}{i}\right\}^2}$$

(w/o derivation (+1))

$$\frac{\sinh(ika)}{i} = \frac{\exp(ika)-\exp(-ika)}{2i} = \sin ka$$

$$T = \frac{1}{1+\dfrac{V_0^2}{4E(E+V_0)}(\sin ka)^2} = \frac{4E(E+V_0)}{4E(E+V_0)+V_0^2(\sin ka)^2} \quad (+3)$$

$\sin ka = 0$, $T=1$ (+2) $\quad ka = n\pi$, $k=\dfrac{n\pi}{a}$, $\dfrac{2\pi}{\lambda} = \dfrac{n\pi}{a}$, $2a = n\lambda$ (+1)

$$k^2 = \frac{n^2\pi^2}{a^2} = \frac{2m(E+V_0)}{\hbar^2}, \quad E = \frac{\hbar^2\pi^2 n^2}{2ma^2} - V_0 \quad (+2)$$

Different way

Total 12 points



c. The tunneling probability T for the left-hand-side case is given in the equation sheet. Please derive the new expression of T for the right-hand-side case, and prove that when $n\lambda=2a$ ($\lambda$ is electron wavelength in the well region, n=1, 2, 3,…), T becomes 100% (resonant tunneling). What are the values of E for these resonant tunneling events? (Please make sure your T expression contains only real parameters, no imaginary parameters, and clearly define your parameters in the expression!)

region I, III $\quad \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0$

region II $\quad \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E+V_0)\psi = 0$ ~~(+1)~~ (+0.5)

(+0.5)

$\psi_I = Ae^{ik_1x} + Be^{-ik_1x} \quad (x < -\frac{a}{2})$ $\quad k_1 = \frac{\sqrt{2mE}}{\hbar}$

~~(+1)~~ $\psi_{II} = Ce^{ik_2x} + De^{-ik_2x} \quad (-\frac{a}{2} \le x \le \frac{a}{2})$ $\quad k_2 = \frac{\sqrt{2m(E+V_0)}}{\hbar}$ (+0.5) ~~(+1)~~

$\psi_{III} = Fe^{ik_1x} + Ge^{-ik_1x} \quad (x > \frac{a}{2})$

no reflected beam (−x direction) in region III, $G=0$ ~~(+1)~~ (+0.5)

① $\psi_I(-\frac{a}{2}) = \psi_{II}(-\frac{a}{2})$

$Ae^{-ik_1\frac{a}{2}} + Be^{ik_1\frac{a}{2}} = Ce^{-ik_2\frac{a}{2}} + De^{ik_2\frac{a}{2}}$ ~~(+0.5)~~ (+0.5)

② $\frac{d\psi_I}{dx}(-\frac{a}{2}) = \frac{d\psi_{II}}{dx}(-\frac{a}{2})$

$Aik_1e^{-ik_1\frac{a}{2}} - Bik_1e^{ik_1\frac{a}{2}} = Cik_2e^{-ik_2\frac{a}{2}} - Dik_2e^{ik_2\frac{a}{2}}$ ~~(+1)~~ (+0.5)

③ $\psi_{II}(\frac{a}{2}) = \psi_{III}(\frac{a}{2})$

$Ce^{ik_2\frac{a}{2}} + De^{-ik_2\frac{a}{2}} = Fe^{ik_1\frac{a}{2}}$ ~~(+1)~~ (+0.5)

④ $\frac{d\psi_{II}}{dx} = \frac{d\psi_{III}}{dx} \quad (at\ \frac{a}{2})$

$Cik_2e^{ik_2\frac{a}{2}} - Dik_2e^{-ik_2\frac{a}{2}} = Fik_1e^{ik_1\frac{a}{2}}$ ~~(+1)~~ (+0.5) eq ① $\times\, ik_1$ + eq ②

$$2Aik_1 e^{-ik_1 a/2} = Ci(k_1+k_2)e^{-ik_2 a/2} - Di(k_2-k_1)e^{ik_2 a/2}$$

eq ③ $\times\, ik_2$ + eq ④

$$2Cik_2 e^{ik_2 a/2} = Fi(k_2+k_1)e^{ik_1 a/2} \qquad C = F\frac{(k_2+k_1)}{2k_2}e^{ik_1\frac{a}{2}}e^{-ik_2\frac{a}{2}}$$

eq ③ $\times\, ik_2$ − eq ④

$$2Dik_2 e^{-ik_2 a/2} = Fi(k_2-k_1)e^{ik_1 a/2} \qquad D = F\frac{(k_2-k_1)}{2k_2}e^{ik_1 a/2}e^{ik_2 a/2}$$

$$2A\cancel{i}k_1 e^{-ik_1 a/2} = F\cancel{i}\frac{(k_2+k_1)^2}{2k_2}e^{ik_1 a/2}e^{-ik_2 a} - F\cancel{i}\frac{(k_2-k_1)^2}{2k_2}e^{ik_1 a/2}e^{ik_2 a}$$

$$(4k_1k_2 e^{-ik_1 a})A = \{(k_2+k_1)^2 e^{-ik_2 a} - (k_2-k_1)^2 e^{ik_2 a}\}F$$

$$F/A = \frac{4k_1k_2 e^{-ik_1 a}}{(k_2+k_1)^2 e^{-ik_2 a} - (k_2-k_1)^2 e^{ik_2 a}} \qquad (+0.5)$$

$$T = \left|\frac{F}{A}\right|^2 = \frac{16k_1^2k_2^2}{|(k_2+k_1)^2 e^{-ik_2 a} - (k_2-k_1)^2 e^{ik_2 a}|^2} \qquad (+0.5)$$

more math . . .

+2

$$T = \frac{4E(E+V_0)}{4E(E+V_0) + V_0^2\sin^2(k_2 a)}$$

+1

$\sin k_2 a = 0$ , $T = 1$

$k_2 a = n\pi$ $\quad k_2 = \frac{2\pi}{\lambda}$ $\quad$ +2

$2a = n\lambda$

$$k_2^2 = \frac{2m(E+V_0)}{\hbar^2} = \frac{n^2\pi^2}{a^2}, \qquad E = \frac{\hbar^2 n^2\pi^2}{2ma^2} - V_0$$

+2