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Exam "Materials Science" (191210740)

October 28th, 2014

General instructions

1) The total time given for this examination is 3 hours (13:45-16:45).
2) Read the complete exam questions before starting, to avoid time problems at the end.
3) It is not allowed to use reference material such as handouts, books or communicating devices (laptops, mobile phones or pda's) during the exam. If needed, lists of formulas, diagrams, tables, etc. will be provided at the exam by the supervisor.
4) Please pay attention to clear writing, the answers should be readable without significant efforts.
5) Students are expected to give detailed and motivated answers. Only complete (not too short) answers with clear drawings (if needed) qualify for the maximum score.

The total mark will be calculated based on:

- Part I: Assignment presentation (25 points max).
- Part II: Answering questions (1-5) of the exam (45 points max).
- Part III: 1st question of choice (15 points max). You can choose one of the questions in the list.
- Part IV: 2nd question of choice (15 points max). You can choose one of the questions in the list.

Good luck!

Part II: Answering questions (1-5) of the exam (45 points max).

Question 1. True or False? Shortly motivate your answer (1 point per question, 10 points max).

1. Semiconductors always exhibit a continuous decrease of their resistivity with increasing temperature.
2. Weakly bonded solids have low melting point, low elastic modulus and high thermal expansion coefficient.
3. Based on thermodynamics one can surely predict if a process can occur at given conditions.
4. Activation energy of a diffusion process is lower at the grain boundaries compared to the bulk.
5. Good wetting can be achieved for a surface having low free-energy when covered with a high free-energy material.
6. The 1st Brullioun zone describes reciprocal space.
7. Measuring decay of polarization in time is usually done to obtain electron-induced polarization.
8. Ferroelectrics are very good dielectrics for using in capacitors.
9. The Bohr radius of a hydrogen atom is 0.529 Å (true); is the 3rd orbit of hydrogen atom then approximately 10^{-12} m?
10. Both film nucleation & growth depend on deposition conditions (pressure, temp., etc.) only.

Question 2. (7 + 3 = 10 points max)

a) In the Ellingham diagram (attached) you can find curves for the following reactions:
   $2C + O_2 \rightarrow 2CO$;
   $2CO + O_2 \rightarrow 2CO_2$;
   $C + O_2 \rightarrow CO_2$.
   Explain origin of the different (i.e. negative, positive and near-zero, respectively) slopes.
b) Explain the difference (if any) between the thermodynamic- and kinetic-based approaches; when can one better use thermodynamics and when – kinetics?

Question 3. (10 points max)

For which of the materials listed below you can expect the largest magnetic moment and why? Which material exhibits the smallest magnetic moment and why?

a) Sc
b) V
c) Mn
d) Fe

Motivate your conclusions with sufficient details.

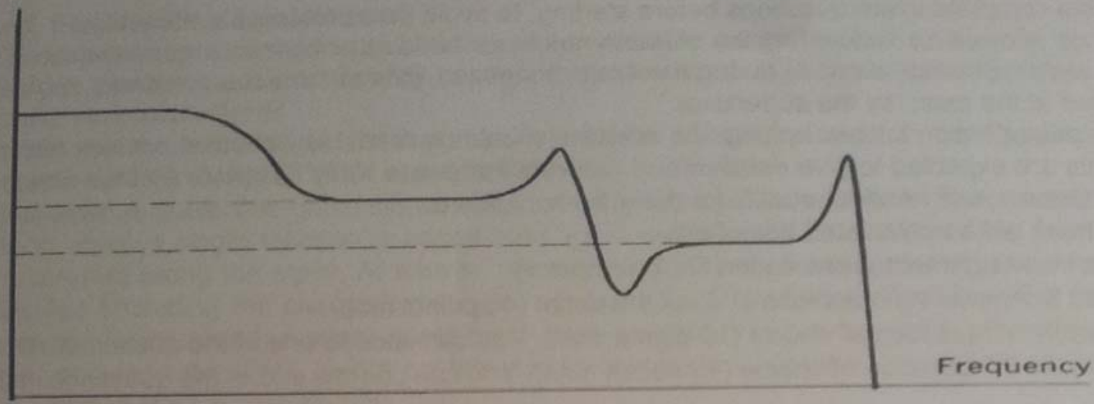
Question 4. (10 points max)

See graph on the next page.

a) What kind of material property you can think of? (1 point)

b) Explain the different parts and all features on this graph. (5 points)
c) What are the corresponding contributing mechanisms? (4 points)

Motivate all your conclusions.



Question 5. (5 points max)

a) We want to design a detector which has to sense radiation at 1500 nm wavelength. What would be a better choice: Si or Ge? Why? Give a short motivation (2 points).
b) Is it true that one can make a laser by using GaAs and not by using Si? Please explain (3 points).

Part III: 1st question of choice (15 points max). Please choose *one* of the questions (6 or 7) below.

Question 6. Phase Change Materials (15 points max)

A. (3 points) Explain the similarities and differences in writing information between a rewritable optical DVD and a Phase Change Memory. Also mention the differences in the material properties that are needed (if any).

B. (3 points) Discuss the similarities and differences for erasing the information. Also mention the differences in the material properties that are needed (if any).

C. The materials discussed are the so-called fast-growth materials: they grow on existing crystalline areas, instead of materials showing nucleation first and then growth. What do you expect to happen when a memory cell with such a material (e.g. PCM-line of 100 nm) is scaled to a next generation where the number of devices per cm^2 will increase by a factor of 2? Assume the thickness of the PCM films to remain the same. Discuss the impact of scaling on the following:

a. (1.5 point) the current needed to write an amorphous bit;

b. (1.5 point) the minimum voltage needed to go from amorphous to crystalline phase;

c. (2 points) your expectation for the stability of the written information (amorphous areas);

d. (4 points) assume the crystallization rate versus temperature is described by an Arrhenius plot with an activation energy of 2 eV. The data (i.e. the amorphous lines) are stable for 10 years at 400 K. How much will the memory lifetime be affected by going to the next generation, assuming nothing else is changed (i.e. only dimensions change)?

Question 7. Materials in Integrated Circuits - ICs (15 points max)

A. (2 points) In general, what is the need to introduce new materials into ICs?
B. (3 points) Compare the metallization schemes for interconnects in e.g. 1995 and 2005 and comment on the differences (if any).
C. (3 points) *Where* and *why* SiO_2 is replaced by HfO_2? Explain with sufficient details.
D. (3 points) Explain the consequences of replacing SiO_2 by HfO_2.

E. (4 points) Explain in your own words what the poly-Si gate depletion means (make corresponding drawing of e.g. a transistor to illustrate), outline the consequences of that on the device performance and give a solution.

Part IV: 2nd question of choice (15 points max). Please choose *one* of the questions (8 or 9) below.

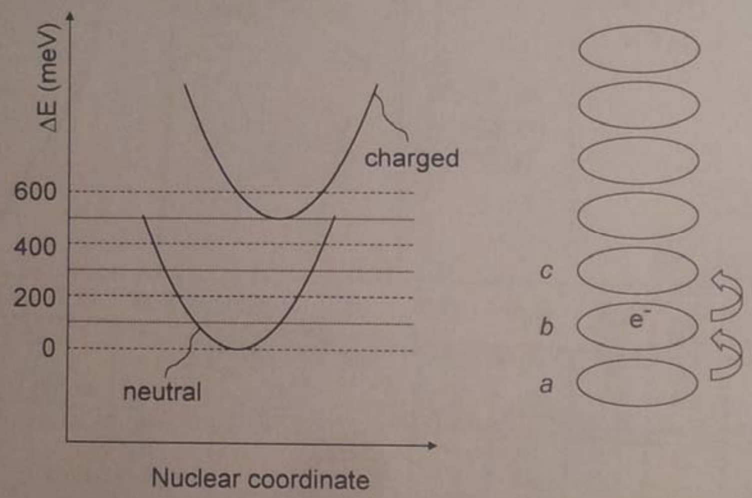
Question 8. Organic Electronics (15 points max)

A. (2 points) Give 3 advantages of organic electronics as compared to inorganic electronics.

B. (3 points) Why is the charge carrier mobility of organic semiconductors in general smaller than that of inorganic semiconductors?

C. (3 points) What are the two parameters that mainly describe charge transport in the hopping regime in organic semiconductors? What about the band-like regime?

D. (3 points) Consider a quasi one-dimensional stack of π-conjugated molecules in their neutral ground state to which a single electron is added (see figure below). The electron can hop from molecule to molecule along the stack. At time t_0, the electron resides on molecule "*a*". Assume that all molecules (including the charged molecule "*a*") are fully relaxed at t_0. Sketch a plot of energy versus the (generalized) nuclear coordinate, such as shown in the figure below on the left-hand side, and indicate which points on the curves represent molecules "*a*" and "*b*" (use labels "*a* at t_0 " and "*b* at t_0" in your sketch).



E. (4 points) At a later time t_1, the electron has <u>just</u> hopped from molecule "*a*" to molecule "*b*". Indicate which points on the curves in your sketch now represent the states of molecules "*a*" and "*b*" (use labels "*a* at t_1 " and "*b* at t_1"). Determine the reorganization energy λ for electron hopping from the plot of ΔE versus the (generalized) nuclear coordinate.

Question 9. Lab-on-chip devices (15 points max)

A. Which materials are widely used to realize lab-on-a-chip devices? Can you explain why these materials are particularly interesting to realize Lab-on-a-chip devices? (*hint*: it can be linked to some of their properties; it can be explained by "historical" reasons, etc). (4 pts)

B. Can you mention at least 3 classes of properties or characteristics which must be considered when choosing materials to realize lab-on-a-chip devices, and justify why they are important? (3 pts)

C. Which material(s) would you recommend to use for the following applications? (explain your choice)

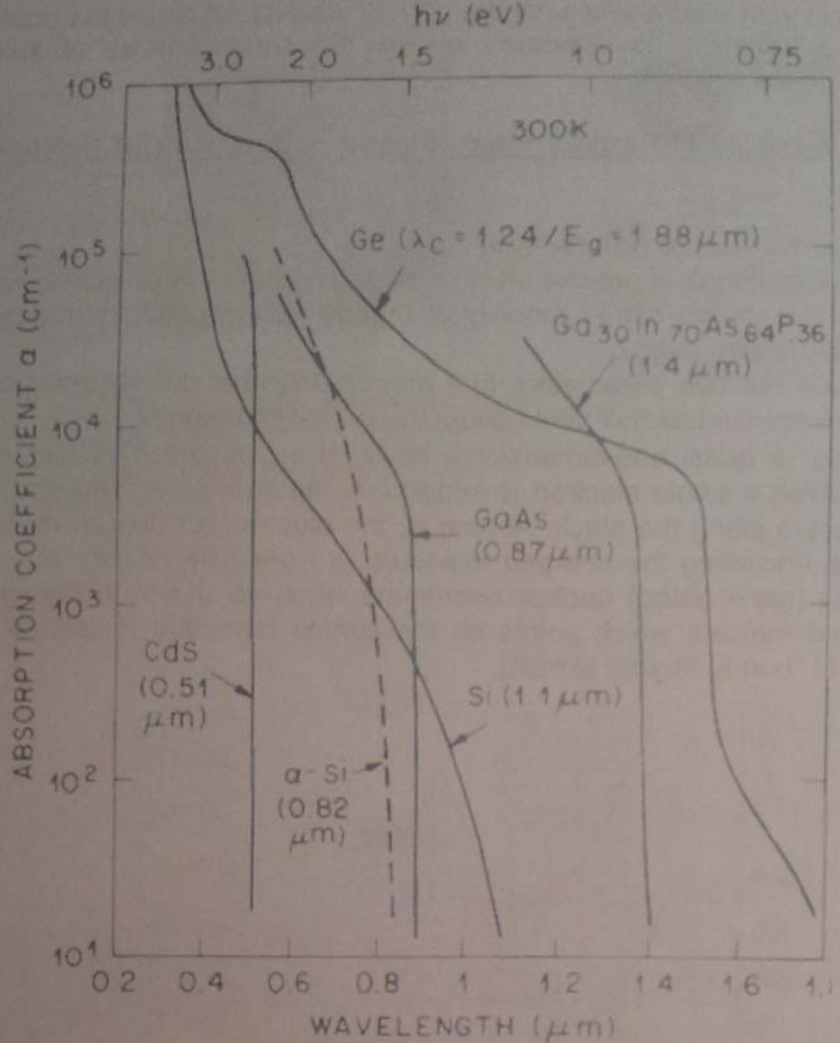
a. For the realization of a microreactor in the field of organic chemistry. (1.5 pts)

b. For the development of user-friendly point-of-care devices with colorimetric readout for poor-resources settings. (1.5 pts)

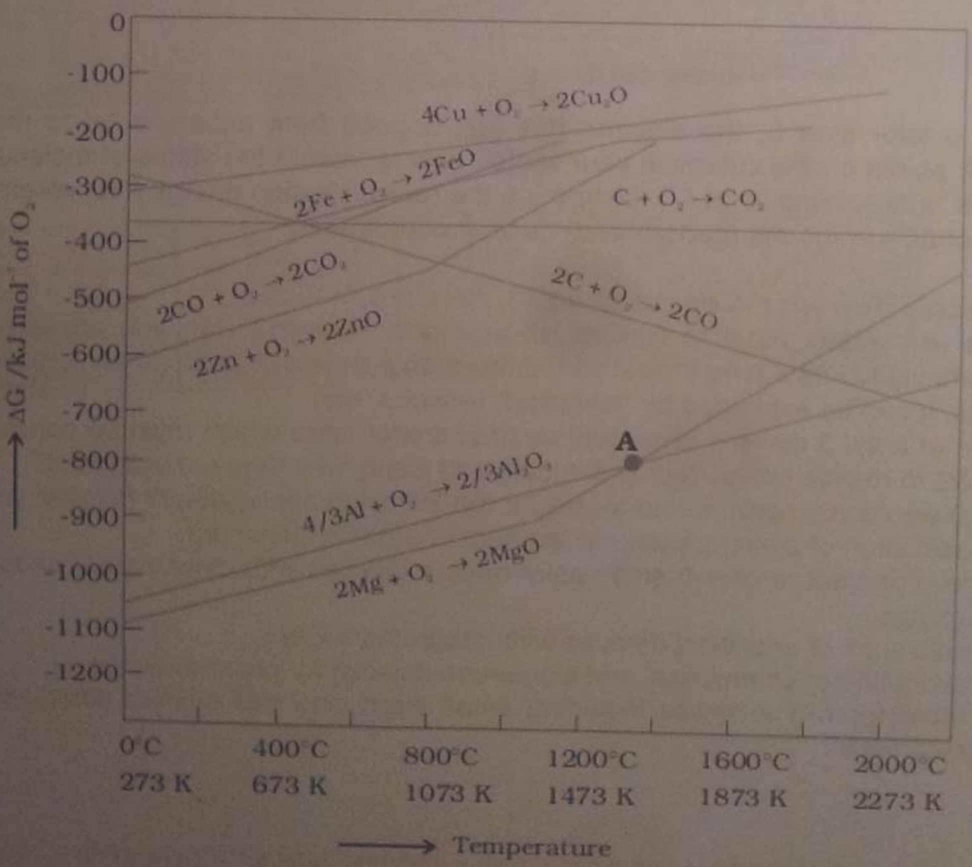
c. For the realization of analytical devices with integrated valves. (1.5 pts)

d. For the fabrication of commercial and single-use devices for blood analysis. (1.5 pts)

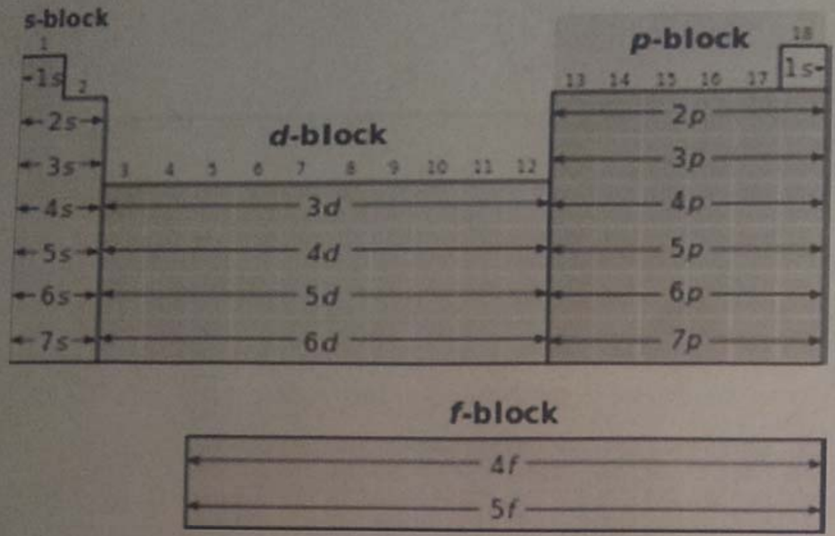
e. For the fabrication of a device including small sized and well-defined structures and with integrated electrodes? (2 pts)



hν (eV)
3.0
2.0
1.5
1.0
0.75
300K
Ge (λc = 1.24/Eg = 1.88 μm)
Ga30In70As64P36
(1.4 μm)
GaAs
(0.87 μm)
CdS
(0.51
μm)
Si (1.1 μm)
a-Si
(0.82
μm)
ABSORPTION COEFFICIENT α (cm-1)
WAVELENGTH (μm)



4Cu + O2 → 2Cu2O
2Fe + O2 → 2FeO
C + O2 → CO2
2CO + O2 → 2CO2
2C + O2 → 2CO
2Zn + O2 → 2ZnO
A
4/3Al + O2 → 2/3Al2O3
2Mg + O2 → 2MgO
ΔG /kJ mol-1 of O2
0°C 273 K
400°C 673 K
800°C 1073 K
1200°C 1473 K
1600°C 1873 K
2000°C 2273 K
Temperature



$1s^2$

$2s^2 2p^6$

$3s^2 3p^6 3d^{10}$

$4s^2 4p^6 4d^{10} 4f^{14}$

$5s^2 5p^6 5d^{10} 5f^{14}$

$6s^2 6p^6 6d^{10} 6f^{14}$

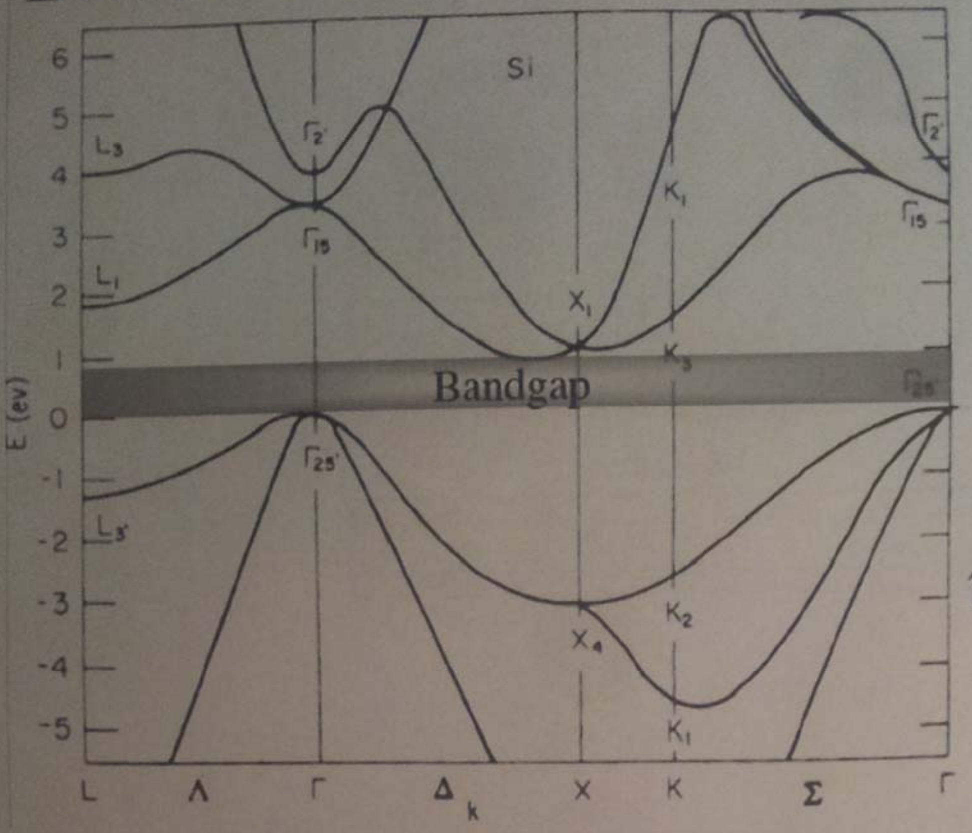
$7s^2 7p^6 7d^{10} 7f^{14}$

s d p

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII			IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
1 H 1.008																	2 He 4.003
3 Li 6.941	4 Be 9.012											5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	10 Ne 20.18
11 Na 22.99	12 Mg 24.31											13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.06	17 Cl 35.45	18 Ar 39.95
19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.90	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.71	29 Cu 63.55	30 Zn 65.38	31 Ga 69.72	32 Ge 72.59	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc 98.91	44 Ru 101.07	45 Rh 102.91	46 Pd 106.4	47 Ag 107.87	48 Cd 112.4	49 In 114.82	50 Sn 118.69	51 Sb 121.75	52 Te 127.60	53 I 126.90	54 Xe 131.30
55 Cs 132.91	56 Ba 137.33	57 La 138.91	72 Hf 178.49	73 Ta 180.95	74 W 183.85	75 Re 186.2	76 Os 190.2	77 Ir 192.22	78 Pt 195.09	79 Au 196.97	80 Hg 200.59	81 Tl 204.37	82 Pb 207.2	83 Bi 208.98	84 Po (210)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra 226.03	89 Ac (227)															

58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm (145)	62 Sm 150.4	63 Eu 151.96	64 Gd 157.25	65 Tb 158.93	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.04	71 Lu 174.97
90 Th 232.04	91 Pa 231.04	92 U 238.03	93 Np 237.05	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (254)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lw (260)

Band structure of Si (diamond)



$$K = \frac{d^2 V}{dx^2}$$

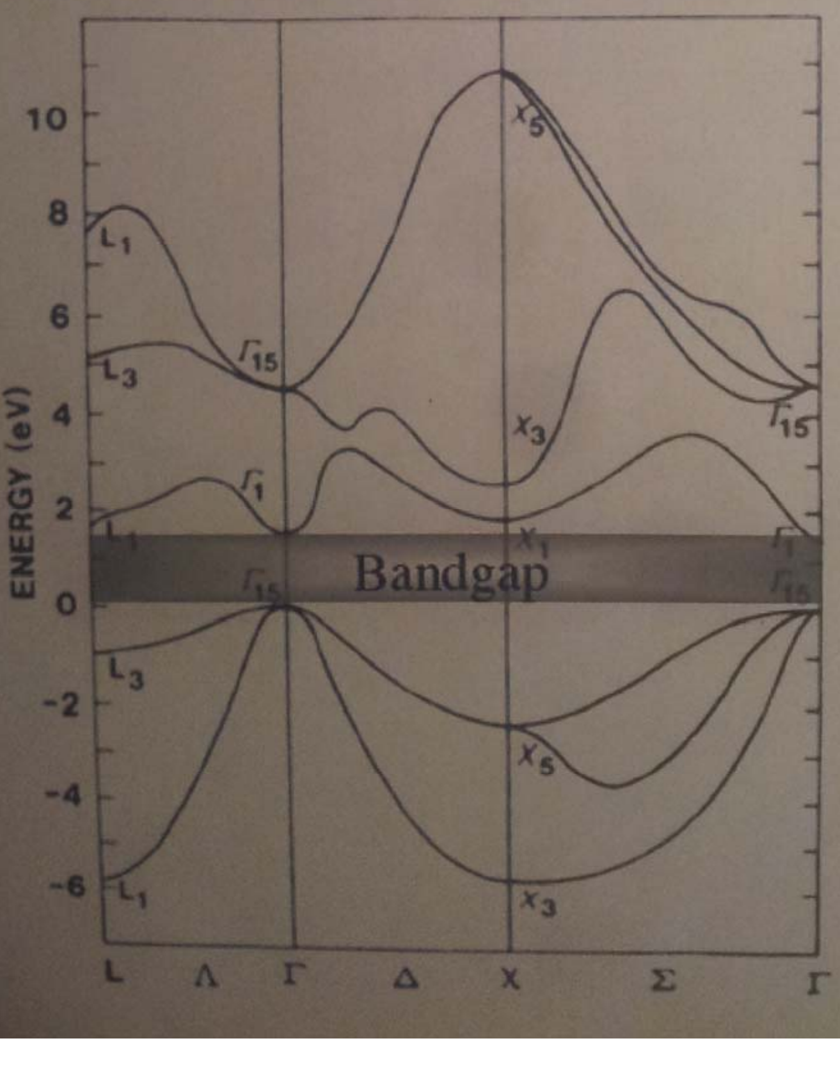
$$=$$

$$\frac{1}{K} = \frac{1}{K_1} + \frac{1}{K_2}$$

$$K = \frac{K_1 \cdot K_2}{K_1 + K_2}$$

$$K = \frac{\frac{Ewt^3}{L_1^3} \cdot \frac{Ewt^3}{L_2^3}}{\frac{Ewt^3}{L_1^3} + \frac{Ewt^3}{L_2^3}}$$

Band structure of GaAs



$$\frac{Ewt^3}{L_2^3 + L_1^3}$$

$$\theta = \frac{TL}{JG}$$

$$\frac{\theta JG}{L} = T$$