MIT3_071F14_ExamISolutio

Name: _____

Amorphous Materials
Exam II
180 min Exam

Problem 1 (30 Points) _____

Problem 2 (24 Points) _____

Problem 3 (28 Points) _____

Problem 4 (28 Points) _____

Total (110 Points) _____

Problem 1

Please briefly justify your choice using ONE sentence.

1) The atoms in an amorphous solid are arranged in a completely random manner without any structural order.

NOT CORRECT

Atoms in amorphous solids possess short range order.

2) Amorphous minerals cannot be found in nature since they are metastable and will eventually crystallize over geological time scale.

NOT CORRECT

e.g. obsidian

3) The mobility gap in amorphous solids is only an empirical fit and has little physical significance.

NOT CORRECT

Mobility gap is well-defined (energies separating localized states from extended states) but difficult to measure experimentally.

4) Terahertz imaging using electromagnetic radiations with frequencies around 1 THz is increasingly becoming a popular imaging technique in security and sensing. At terahertz frequencies, electrons rather than ions contribute to dielectric permittivity due to their small mass.

NOT CORRECT

1 THz (corresponding to 300 μm in wavelength) is much lower than the characteristic vibrational frequencies of most atomic bonds.

5) In amorphous silicon solar cells, the photo-generated electrons and holes are transported to the electrodes primarily via the hopping mechanism.

NOT CORRECT

Extended state conduction is the primary pathway for charge transport since: 1) a good solar cell requires H-passivation which leaves behind few defects; and 2) it is far more efficient.

6) Pyrex® kitchenware sold in the States nowadays is not recyclable as they are made of borosilicate glasses.

NOT CORRECT

Pyrex glassware sold in the US nowadays are made of tempered soda-lime glass.

7) Amorphous metals are difficult to obtain due to the non-directional nature of metallic bonds. As a result, they can only be prepared using melt spinning, laser melting or vapor deposition.

NOT CORRECT

Bulk metallic glasses can be prepared using casting.

8) Low iron soda-lime glasses are used in building structures such as the Grand Canyon Skywalk due to their reduced risk of spontaneous breakage.

NOT CORRECT

High optical transparency is the reason for using low iron glass.

9) Area under DTA curves equals to the heat absorbed or released during a phase transition.

NOT CORRECT

There is no simple analytical relation between heat absorbed or released during a phase transition and the area under DTA curves (note that the

equation $T_S - T_R = \frac{1}{K}\frac{dT}{dt}\cdot(C_R - C_S)$ only holds for steady state, i.e. regions w/o phase transition in a DTA scan).

10) Glasses obtained through rapid cooling exhibit larger molar enthalpy compared to glasses of the same composition obtained through slow cooling.

CORRECT

The H-T diagram is universal for glasses.

Problem 2

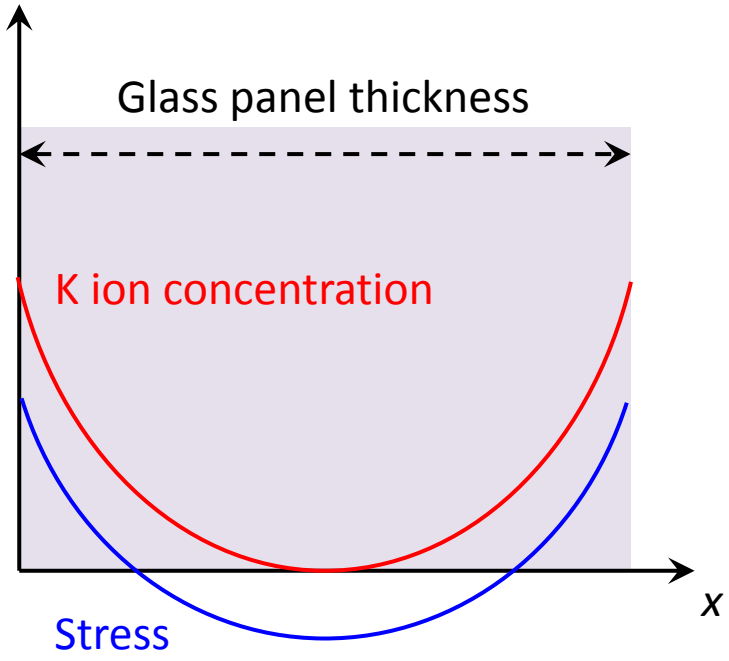
1) Do you agree with the following statement: "glass is basically a liquid with very high viscosity"? Please justify your answer.

Solution:
Yes and no – glass (well below T_g) does exhibit high viscosity, although from a rheological perspective it cannot be described using an ideal viscous liquid model since it is viscoelastic. Structurally glass is also different from the high-temperature supercooled liquid state as well, as is evident from their different coefficient of thermal expansion and heat capacities.

2) Consider a chemical strengthening process for thin sodium aluminosilicate glass laminates. With prolonged potassium salt bath, the case depth can increase to half of the laminate thickness. Schematically plot the potassium ion concentration depth profile and the internal stress distribution in the glass laminate. Briefly explain your reasoning.

Solution:

Note that area under the stress profile has to be zero due to force equilibrium.



3) Explain why structural relaxation is most pronounced in glasses near the glass transition regime.

Solution:
When $T >> T_g$, relaxation is short compared to observation time, and thus the glass forming liquid always stays in a quasi-equilibrium state. When $T << T_g$, relaxation is very long compared to observation time, and negligible relaxation occurs during experiments. Only when $T \sim T_g$, the Debroah number is close to unity and relaxation becomes pronounced.

Problem 3

Your advisor gave you a vacuum thermally evaporated thin film silicon sample and asked you to identify if the sample is amorphous or polycrystalline. You decided to first look into X-ray diffraction and the following table is what you found from the powder diffraction database for silicon.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C Internal standard W, a = 3.16524 Å			
d(Å)	I	hkℓ	2θ(°)
3.13552	100	111	28.443
1.92011	55	220	47.303
1.63747	30	311	56.123
1.35772	6	400	69.131
1.24593	11	331	76.377
1.10857	12	422	88.032
1.04517	6	511	94.954
0.96005	3	440	106.710
.91799	7	531	114.094
.85870	8	620	127.547
.82820	3	533	136.897

a) Schematically plot the X-ray diffraction spectra of a large-grain polycrystalline silicon sample and an amorphous silicon sample.
b) Schematically plot the pair distribution functions of a large-grain polycrystalline silicon sample and an amorphous silicon sample. Please clearly label what the axes represent in your plot.
c) In a polycrystalline material, what happens to its X-ray diffraction peaks when the crystal grain size decreases? Why?
d) The XRD spectrum you obtained from the sample consists of broad diffraction peaks, making you wonder if the sample is nanocrystalline or amorphous. Can you design an experiment to find it out?
e) You identified that the film is amorphous. Now your advisor wants you to make a high-efficiency solar cell out of it. Do you think the idea will work? Why?
f) Can you propose one or more methods to improve the performance of your solar cell device (so that you can graduate on time)?

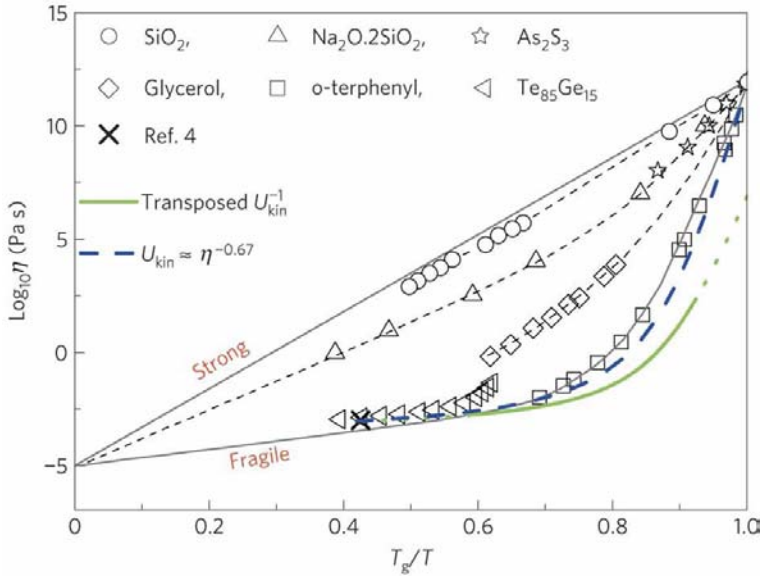
Solution:
c) Restriction of periodicity in the real space leads to broadening of diffraction peaks in the reciprocal space (Scherrer equation).

d) Selective area electron diffraction. Thermal analysis is a possible alternative although analysis of thin film samples is challenging.

e) No. Thermally evaporated a-Si films contains high concentrations of dangling bond defects which leads to Fermi-level pinning and also enhances carrier recombination.

f) H-passivation, for example via annealing in hydrogen or hydrogen plasma treatment.

Problem 4

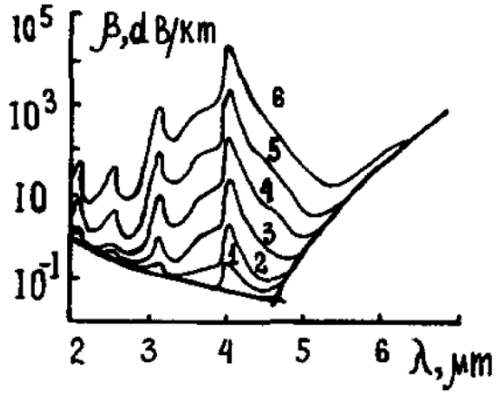


After spending your time at school working on a-Si solar cells, you decided to look for changes and moved to a company specializing in glass optics. You are provided the plot above.

a) Explain the structural difference between strong and fragile glass forming liquids.

b) Which glass composition is easier to be drawn into a fiber, SiO_2 or As_2S_3? Why?

c) The following figure shows the optical loss spectra in As_2S_3 optical fibers with increasing hydrogen impurity concentration (from 1 to 5) calculated by one of your colleagues. Label the optical attenuation mechanisms contributing to the fiber optical loss in the figure and mark the wavelength regimes where each mechanism is most pronounced.



d) In As_2S_3 glass far from equilibrium (e.g. glass formed by vapor condensation), the following equilibrium exists:
$2As_2S_3 \leftrightarrow As_4S_4 + (2/x)\ S_x$
What do you think is the impact of this chemical transformation on the material's optical loss?
e) As_2S_3 is a common material for infrared optics given its low loss. The following photo shows As_2S_3 infrared lens pieces produced by your company. You wonder why does the glass exhibits a red/yellow color?

f) As_2S_3 glass infrared lenses can be fabricated using a precision glass molding process at a viscosity value of ~ 10^7 Pa·s. Estimate the molding temperature of As_2S_3 glass lenses.
g) Suppose you would like to decrease the molding temperature of As-S glass lenses by tuning the glass stoichiometry to minimize mold sticking. What composition(s) would you choose? Why?

Solution:
a) Structures of strong liquids do not change over the temperature range and thus exhibit the same activation energy. The structural units of motion in fragile liquids vary as temperature changes, and as a result the same activation energy also changes.

b) SiO_2. Fiber drawing needs to be performed at a specific viscosity value to ensure uniformity. Strong liquids are less susceptible to temperature variation and also have a wider fiber drawing viscosity window.

d) The reaction leads to phase segregation and increased Rayleigh scattering.

e) The optical bandgap of As_2S_3 is ~ 2.3 eV (~ 530 nm), and therefore only orange and red color light can transmit through the glass.

g) A sulfur rich composition is favorable as it decreases network connectivity and reduces viscosity.

3.071 Amorphous Materials

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