Advanced Vitreous State - Charge Conduction in Glass Problem set

This problem set can be done collaboratively among yourselves. Consider that you are all on a research team and working together to solve these problems. Share what you learn with others in ways that you think helpful. Face book, You tube, email... etc. Do your part and work collaboratively, don't sit back and wait for the answers to come, this type of work is not collaboration, it is copying. Work on the problems and share what you've done. Use Teamwork. When you are done, write a brief summary of the effect collaborating had on your success in this project, the nature and manner of the ways you collaborated (what web/electronic tools you sued) and then attach links to all sharing sites, tools etc that you used. If done, collaboratively, I would expect all of you to get perfect scores on this problem set. Each person is responsible to turning in the answers to the problems, just like you would for the other HWs, this time you just get to work together.

You can use the Adobe web site to post stuff as well as to meet interactively and share learning.

Due December 11, which is among the reasons it can be done collaboratively.

- 1. Show using SI units that $\sigma = 1/\rho \equiv neZ\mu$ in this equation is consistent with the units described on page 10 of the Part 1 Lecture
- 2. Show that the units of the pre-exponential factor σ_0 in the equation below are consistent with the units of the conductivity given above:

$$\sigma(T) = \frac{n v_0 \lambda^2 (ze)^2}{RT} \exp\left[-\frac{\Delta E_{act}}{RT}\right] \equiv \frac{\sigma_0}{T} \exp\left[-\frac{\Delta E_{act}}{RT}\right]$$

- 3. Now using nominal values for n_0 , v_0 , and λ calculate the expected range of values for σ_0 expected from the equation given in problem 2 above for Na, K, and Cs alkali silicate glasses at a mole fraction of M₂O ~25-35 mole%. How do these values compare to the values of σ_0 extrapolated from the figure on slide 17 of the Part 1 lectures and other values obtained from the literature?
- 4. Now, consider the strain energy ΔE_s , as described in Part 2 of the lectures and equation 14.35 in your book. Calculate estimated values for the door way radius, r_D ,

assuming that the small cation, Na, is in tetrahedral coordination and the larger cations, K and Cs, are in octahedral coordination by oxygen in alkali silicate glasses. at a mole fraction of $M_2O \sim 25$ -35 mole%. You can find M+ radii and O- radii in the literature as a function of coordination. Assume the cation jumps through one of the faces of the tetrahedral or octahedral sites. How do these estimated values for the doorway radii for the different glasses compare to the radii of the cations?

Now using these values and values for the shear modulus G, the cation radius, r_c , calculate the strain energies you would expect for Na, K, and Cs cations in one alkali silicate glass at a mole fraction of M₂O ~25-35 mole%. Describe what this trend tells you about the behavior of alkali ion conductors as a function of alkali radius.

- 5. Now, consider the coulomb energy, ΔE_C , as described in Part 2 of the lectures and equation 14.34 in your book. Use appropriate values for the cation and oxygen anion charge and radii and assume that r_e is the jump distance $\lambda/2$ can be calculated from the nominal cation number density, and calculate ΔE_C for Na, K, and Cs alkali silicate glasses at a mole fraction of M₂O ~25-35 mole%.
- 6. Communicate among yourselves and share literature values that you all can find for the conductivity and activation energies for Na, K, and Cs alkali silicate glasses at a mole fraction of M₂O ~25-35 mole%. Compare the values you obtain from the literature to the values for the pre-exponential factor and total activation energy (sum of ΔE_C and ΔE_s) calculated in Problems 3, 4 and 5 above. What can you say about the accuracy of the calculations? Can you describe ways in which the accuracy might be improved?
- Write a brief summary of the effect collaborating on this project had on the success in developing answers to the questions. Was it more helpful, less helpful, faster, slower, you learned more, you learned less....etc.
- 8. Write a brief summary of what collaboration tools you used to share learning on this problem set, web sites, links, collaboration software... etc.