

1. Explain why electronic doping by introduction of suitable donor/acceptor levels in an amorphous material is difficult.

Electronic doping is difficult in amorphous materials due to the high concentration of intrinsic states in the gap [1]. When dopants are added, the concentration of introduced states is low compared to the intrinsic states, making it difficult to move the Fermi level. Additionally, with their low coordination number and flexibility, amorphous materials can undergo relaxation when dopants are added [2]. This traps the added charge carriers instead of producing a system with more free carriers. This can be modeled with VAPs, which can use the added carriers to change the charge of their dangling bond [3]. To introduce a large enough number of states to move the Fermi level, the number of dopants must be at least double the number of VAP defects [3].

---

2. Explain why the doping discussed in problem (1) might not improve carrier mobility.

Doping introduces charged defects,  $D^+$  and  $D^-$ , and though these defects are only capable of trapping either electrons *or* holes respectively, they are much more effective trap sites than  $D^0$  [4]. Street et al. found  $D^+$  centers were 5 times more effective than  $D^0$  centers at trapping electrons and  $D^-$  centers were 2-4 times more effective at trapping holes than  $D^0$  centers. Similarly, Kazakova and Tsandin [5] found that when the number of dopants is 2 to 3 times the number of defect centers, hole mobility decreases as dopant concentration increases.

---

3. Would you expect to see blocking contacts in a metal-amorphous semiconductor contact? Explain your answer.

I would expect to see blocking contacts because of the high concentration of trap states in an a-semiconductor. Until these traps are filled, one would observe an ohmic contact at low voltages  $< 10V$  [6]. However, once the states are filled, a-semiconductors exhibit space charge limited conduction (SCLC) [6, 7, 8] where carriers from the metal can only enter states in the semiconductor as carriers move from those states. High voltages ( $10^4 V/cm^2$ ) are then needed to overcome SCLC and reach superohmic behavior [6, 7].

---

4. Describe the structural order giving rise to extended (delocalized) states and localized states in an amorphous semiconductor.

Localized states can come from defects like VAPs while extended states consist of the more stable “happy” charge carriers. Drabold et al. [9] describe this quantum mechanically by considering “severe distortions” or the bonds that deviate the greatest from a tetrahedral structure in the case of a-Si. As larger distortions are less likely to occur, there is less degeneracy and especially so if those distorted clusters are isolated. As distortions become

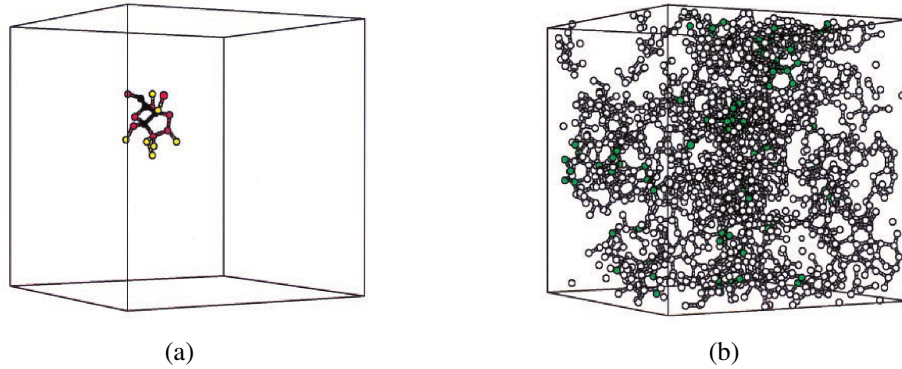


Figure 1: Selected results from Drabold et al. [9] of structure contributing to (a) midgap states and (b) extended states. Color represents charged regions.

less severe, they are more likely to occur and lead to mixing of states. This was seen by mapping energy resolved states (e.g. near the Fermi level, at the valence band tail, etc.) to the structure. Near the Fermi level the authors found charge localized to a small cluster exhibiting very high distortion (**Fig. 1(a)**). As they shifted the energy window towards the valence band the cluster became larger. Finally, when examining the deep valence band states the charge mapped to several small clusters (**Fig. 1(b)**). In short, localized states originate in regions with the greatest structural disorder, while extended states come from regions of “ideal” structure, in this case tetrahedral.

5. Provide definitions/explanations of the following:

- Hubbard correlation energy

Correlation energy is the energy between opposite spin electrons. Hubbard first identified this repulsion present in systems with strongly localized orbitals, such as transition metals and actinides [10].

- Localization length

The localization length is the rate of exponential decay of the eigenstate as position goes to infinity [11].

- Anderson transition

The Anderson transition describes the change from localized states in the band gap to extended or delocalized states. [9]

- Localized “in the Anderson sense”

Localized states are where no transport occurs or no quantum jumps between sites [12].

6. (a) What is the difference between variable range hopping and nearest neighbor hopping?  
 (b) In which type of conduction will tunneling occur?

Nearest neighbor hopping is thermally activated, while at low temperatures carriers will follow variable range hopping where the jump is selected based on the greatest probability of success [13]. Tunneling will occur in variable range hopping because there is little thermal energy for phonon assisted hopping.

## References

- [1] J. Tauc, Amorphous semiconductors, *Physics Today* 29 (1976) 23–31. doi:10.1063/1.3024406.  
URL <http://physicstoday.scitation.org/toc/pto/29/10>
- [2] J. Kim, H. Hiramatsu, H. Hosono, T. Kamiya, Effects of sulfur substitution in amorphous InGaZnO 4 : optical properties and first-principles calculations, *Journal of the Ceramic Society of Japan* 123 (7) (2015) 537–541. doi:10.2109/jcersj2.123.537.
- [3] H. Fritzsche, Why are chalcogenide glasses the materials of choice for Ovonic switching devices?, *Journal of Physics and Chemistry of Solids* 68 (2007) 878–882. doi:10.1016/j.jpcs.2007.01.017.
- [4] R. A. Street, J. Zesch, M. J. Thompson, Effects of doping on transport and deep trapping in hydrogenated amorphous silicon, *Applied Physics Letters* 43 (672) (1983) 672–674. doi:10.1063/1.94441.  
URL <http://aip.scitation.org/doi/10.1063/1.94441>
- [5] L. P. Kazakova, K. D. Tsendin, Controlling the U-center density in Se-As chalcogenide-glass semiconductors by doping with metals and halogens, *Semiconductors* 33 (7) (1999) 795–798. doi:10.1134/1.1187784.  
URL <https://link.springer.com/content/pdf/10.1134/1.1187784.pdf>
- [6] R. Singh, S. K. Tripathi, S. Kumar, Space charge limited conduction in a-(Ge<sub>20</sub>Se<sub>80</sub>)<sub>1-x</sub>Sn<sub>x</sub> thin films, *Journal of Non-Crystalline Solids* 352 (2006) 3230–3235. doi:10.1016/J.JNONCRYSQL.2006.05.015.  
URL <https://www.sciencedirect.com/science/article/pii/S0022309306006855>
- [7] V. Kushwaha, A. Kumar, Space charge limited conduction in bulk Se<sub>100-x</sub>Sb<sub>x</sub> chalcogenide glasses, *Materials Letters* 60 (17-18) (2006) 2148–2152. doi:10.1016/J.MATLET.2005.12.090.  
URL <https://www.sciencedirect.com/science/article/pii/S0167577X05013510>
- [8] M. A. Majeed Khan, M. Zulfequar, M. Husain, Study of density of localized states of a-Se<sub>80</sub>Te<sub>20-x</sub>Pb<sub>x</sub> films by space charge limited conduction measurements, *Materials Letters* 57 (2003) 2894–2900. doi:10.1016/S0167-577X(02)01393-9.  
URL [www.elsevier.com/locate/matlet](http://www.elsevier.com/locate/matlet)
- [9] D. A. Drabold, U. Stephan, J. Dong, S. M. Nakhmanson, The structure of electronic states in amorphous silicon, *Journal of Molecular Graphics and Modelling* 17 (2000) 285–291.  
URL <https://pdfs.semanticscholar.org/fb3e/2ef301f3809ddf6a977296bf2f748a70dfb5.pdf>

- [10] J. G. Lee, Computational materials science : an introduction, CRC Press, 2012.  
URL <https://www.crcpress.com/Computational-Materials-Science-An-Introduction/Lee/p/book/9781439836170>
- [11] S. Derevyanko, Anderson localization of a one-dimensional quantum walker, Scientific Reports 8 (1) (2018) 1795. doi:10.1038/s41598-017-18498-1.  
URL <http://www.nature.com/articles/s41598-017-18498-1>
- [12] P. W. Anderson, Absence of Diffusion in Certain Random Lattices, Physical Review 109 (5) (1958) 1492–1505.
- [13] Z. G. Yu, X. Song, Variable Range Hopping and Electrical Conductivity along the DNA Double Helixdoi:10.1103/PhysRevLett.86.6018.  
URL <https://journals.aps.org/prl/pdf/10.1103/PhysRevLett.86.6018>