Computational Methods for Amorphous Semiconductor Devices

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Abstract

- DOS
- structural modeling

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1. Introduction

2. Density of States

Raty 2015 [1]

- Motivation
  - ”Amorphous materials are out of thermodynamic equilibrium”
  - subject to physical aging
  - phase-change materials (PCMs) have a fast, reversible switch between a conductive crystalline and more resistive amorphous phase
  - aging increases the resistivity - ‘resistance drift’
  - computer simulation to investigate relaxation processes
  - **Modeling comment:** complexity of the chemistry requires DFT to describe and understand bonding and the amorphous phase
- Literature
  - DFT simulations of GeSbTe alloys report many tetrahedrally bonded Ge, which does not exist in crystal. These are obtained from MQ calcs
- Methods
  - Car-Parrinello
  - **To circumvent time scale problem, generated collection of a-structures**
  - mixed Gaussian/plane wave code in CP2K
  - cutoff 300 Ry

- sampled at gamma only
- annealed using plane-wave code in Quantum Espresso
- 34 Ry
- 3.84 fs
- Berendsen thermostat
- 10 models produced starting from liquid

- Results
  - Ge^T is associated with homopolar Ge-Ge bonds
  - heat of formaion shows homopolar bonds more favorable in GeTe than GeSe and SnTe
  - wanted to investigate effects of varying amounts Ge-Ge bonds
  - used different alloys along the phase diagram and substituted with Ge or Te to form different GeTe structures ”mimicking aging”
  - homopolar bonds correlated with tetrahedral Ge
  - freezing at density of amorphous GeTe, tetrahedral rich models had the largest values of stress
  - this agrees with experiments showing the drift of PCMS is accompanied by stress relief
  - order parameter d_4/d_0 goes from tetrahedrally bonded Ge, Ge^T, to Ge^{III} and d_3/d_0 goes from Te^{II} to Te^{III}
  - increase in band gap directly linked to decrease in homopolar bonds
  - ”melt-quenched model has a smaller band gap and possesses a (localized) mid-gap state”

References

[1] J. Y. Raty, W. Zhang, J. Luckas, C. Chen, R. Mazzarello, C. Bichara, M. Wuttig, Aging mechanisms in amorphous phase-change materials, Nature Communications 6 (7467) (2015) 1–8. doi:10.1038/ncomms8467.
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