COMBINING FIRST PRINCIPLES SIMULATIONS, TOPOLOGICAL CONSTRAINT THEORY, AND EXPERIMENTS TO OPTIMIZE OTS CHALCOGENIDE ALLOYS

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Ovonic threshold switches (OTS) based on amorphous chalcogenide alloys have emerged as leading candidates for selectors in non-volatile memory applications. The low OTS leakage current prevents sneak paths and unintentional memory cell selection. Above the threshold voltage, OTS experiences a volatile transition to a high conductivity state and provides sufficient current to switch the neighboring memory element. Given the broad interest in the switching mechanism and the nature of defects in chalcogenide glasses, there is a clear need to understand how material properties change with composition. We will highlight our work using topological constraint theory, density functional theory, and insight from experiments to identify key trends in thermal and electronic properties of chalcogenide alloys. In particular, we will show that tailoring the atomic network in Si_xTe_{1-x} glasses can lead to localization of over 40% of the vibrational modes and ultralow thermal conductivity (~0.1 W/mK)[1]. Using topological constraint theory, we can link this ultralow thermal conductivity to a transition from an over-constrained (rigid) to under-constrained (floppy) atomic network for Te rich alloys. Topological constraint theory also provides a natural language to characterize the properties of multi-element chalcogenide alloys. We find that selector threshold voltage and leakage current exhibit clear trends with the mean coordination number and that this metric can be used to optimize materials[2]. Finally, given the high fields and temperatures experienced during operation, OTS/electrode interfacial interactions can significantly affect long-term device endurance. We have developed machine learning potentials[3,4] to examine interactions between GeSe alloys and Ti electrodes. Our long-term (>1 ns) molecular dynamic simulations[7] using these potentials shows significant interdiffusion at the Ti|GeSe interfaces. We will discuss the impact of interdiffusion on device performance.

Keywords: Chalcogenide alloys, Topological constraint theory, Phase Change, Ovonic Threshold Switch.
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References

[1] K. Aryana, D. A. Stewart, J. T. Gaskin, J. Nag, J. C. Read, D. H. Olson, M. K. Grobis, P. E. Hopkins, "Tuning network topology and vibrational mode localization to achieve ultralow thermal conductivity in amorphous chalcogenides", Nature Communications 12, 2817 (2021).
[2] J. C. Read, D. A. Stewart, J. W. Reiner, B. D. Terris, "Evaluating Ovonic Threshold Switching Materials with Topological Constraint Theory", ACS Applied Materials and Interfaces 13, 37398 (2021).
[3] A. V. Shapeev, "A Class of Systematically Improvable Interatomic Potentials", Multiscale Modeling and Simulation 14, 1153 (2016).
[4] S. Smidstrup et al., "QuantumATK: an integrated platform of electronic and atomic-scale modelling tools", Journal of Physics: Condensed Matter 32, 015901 (2020).
[5] V. A. Venugopal, G. Ottaviani, C. Bersolin, D. Erbetta, A. Modelli, "Thermal stability of $Ge_2Sb_2Te_5$ in contact with Ti and TiN", Journal of Electronic Materials 38, 2063 (2009).
[6] J.-L. Battaglia, A. Kusiak, A. Saci, R. Fallica, A. Lamperti, "Effect of a thin Ti interfacial layer on the thermal resistance of $Ge_2Sb_2Te_5$-TiN stack", Applied Physics Letters 105, 121903 (2014).
[7] J. Scheider et al., "ATK-ForceField: a new generation molecular dynamics software package", Modeling Simul. Mater. Sci. Eng. 25, 085007 (2017).