

Glass transition temperature of chalcogenides predicted by large neural network models

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Abstract: Chalcogenide glasses are versatile and complex amorphous inorganic materials with exceptional mechanical, thermal and optoelectronic properties. Among their modern technological applications is the integration in storage class memory devices as both phase change memory (PCM) and ovonic threshold selector components (OTS) [1]. The current research is undergoing the transition from the binary 1PCM-1OTS architecture to more performant and scalable selector-only memory structure. The thermal stability against high temperatures is one important requirement for the selector component, ensuring the maintenance of its structural and electrical properties across repeated and prolonged thermal stress [1]. Glass transition is a fundamental glass property taking place in a narrow temperature interval upon incremental heating. It is defined as the endothermic structural transformation from rigid solid glass to viscous supercritical liquid at the viscosity threshold of $\sim 10^{12}$ Pa·s and it depends on chemical composition, topological network structure, and heating rate. In this work we build and optimize a complex deep neural network (DNN) trained and tested on glass compositions collected from the SciGlass database [2]. The input features represent statistical functions derived from fundamental physico-chemical attributes of the constituent elements, enabling the model to capture underlying physically meaningful compositional patterns. The robustness of the model was further validated on an additional set of 124 chalcogenide glasses from chemical systems not present in the training set, including compositions with elements absent from the SciGlass collection. We compared our specialized DNN with the multitarget neural network GlassNet [3], currently the largest open model for general glass property prediction. Prediction results showed that our model significantly outperformed GlassNet, achieving a root mean squared error of 38.44°C compared to 99.64°C, due to the ability to generalize to compositions with unseen elements where GlassNet has limitations. Our specialized model provides a reliable, composition-driven tool for rapid screening of chalcogenide glass compositions relevant to memory device applications.

Keywords: Chalcogenide glasses, Glass transition temperature, Deep neural networks

References

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