

High-throughput machine learning-guided exploration of chalcogenide materials for resistive switching devices

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Abstract: Chalcogenide glasses have emerged as promising candidates for neuromorphic computing and resistive switching memory devices due to their unique electronic properties and structural flexibility. However, traditional materials discovery approaches are time-consuming and resource-intensive, limiting exploration of the vast compositional space available in these systems. Machine learning (ML) combined with high-throughput (HT) experimental techniques offers a paradigm shift in accelerating the discovery of novel functional materials with targeted properties.

The first step was to establish guiding principles for composition selection. A composition map for ovonic threshold switching (OTS) materials was constructed based on elemental bonding and topological parameters, organizing the Te-based chalcogenide phase space into regions of varying switching probability. Compositions selected from different areas of the map were synthesized and electrically characterized in nanoscale devices, confirming OTS behavior [1]. While map-guided synthesis provides targeted access to individual compositions, covering broad multi-element regions requires a different approach. Magnetron co-sputtering from multiple targets enables the simultaneous synthesis of continuous compositional libraries. Applied to the Si-Ge-Te system, a single combinatorial deposition run covered a broad ternary compositional range, and systematic structural and optical characterization across the library uncovered amorphous compositions beyond the bulk glass formation domain [2].

The compositional and property data generated by combinatorial synthesis provided the foundation for introducing ML into the discovery workflow. An ensemble ML classifier trained on a database of more than 30k chalcogenide compositions using physics-inspired descriptors derived from topological constraint theory, thermodynamic, and elemental attributes achieved ~89% classification accuracy. Combinatorial synthesis data provided experimental validation for the predictions. Applying the same ML framework to optical properties, a model for refractive index prediction was trained on a small dataset of glass compositions, achieving $R^2 = 0.90$ [3]. The Si-Ge-Te thin films prepared by combinatorial sputtering served as an independent experimental validation set.

Combinatorial synthesis and ML prediction are not independent efforts, they are interconnected. HT experiments provide the training data and experimental validation for ML models, while ML predictions direct synthesis toward the most promising compositional regions, reducing the number of experiments required to identify functional materials for resistive switching and selector applications.

References

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