Data-Driven Design of Multi-Element Thermal Insulating Thin Films for Advanced Thermal Management

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ABSTRACT

The design of thermal insulating coatings for advanced energy and electronic applications requires a deep understanding of both intrinsic and interfacial thermal transport. In this study, we present a data-driven workflow that integrates interfacial thermal resistance (ITR) modeling, low thermal conductivity screening, and inverse materials design for thin-film applications.

We first introduce our previously developed ITR prediction framework, built upon a curated experimental ITR database [1] and machine learning models [2], which enables the estimation of ITR based on interfacial chemical and structural information. Using this framework, we designed thermal insulating thin films with ultra-low thermal conductivities [3,4].

Building on this foundation, we developed predictive models for bulk thermal conductivity using periodic descriptors [5], trained on inorganic compounds from the AtomWork-Adv. (AWA) database [6]. These compact and chemically meaningful descriptors enable efficient learning, achieving a prediction accuracy of R^2 ~0.8 for bulk thermal conductivity. Applying these models, we screened over 150,000 known materials in AWA and explored potential multi-element (>5) compositions for low thermal conductivity. While none of the screened materials fully satisfied practical constraints such as non-toxicity and low cost, the approach identified unexplored compositional systems worthy of further investigation.

Experimental validation of these candidates is currently underway in collaboration with thin-film fabrication teams. This integrated pipeline—combining ITR modeling, bulk thermal property prediction, and multi-element composition design—offers a promising pathway toward the development of next-generation thermal management materials.

Keywords: thermal insulating films, thermal conductivity, periodic descriptors, multi-element materials

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