Revolutionizing Electronics with Advanced Interfacial Heat Management

Yen-Ju Wu

National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan. e-mail: Wu.YenJu@nims.go.jp

In the rapidly advancing field of electronics, managing heat dissipation effectively is more critical than ever. As devices become increasingly powerful and compact, the challenge of efficient heat management intensifies. Interfacial heat transport plays a pivotal role in this process, requiring innovative solutions and accurate predictive models to ensure the reliability and performance of electronics.

Efficient heat dissipation is essential to maintain the performance and longevity of electronic devices. Interfaces between different materials in a device often become bottlenecks for heat flow, leading to overheating and potential failure. Interfacial thermal resistance (ITR) measures the resistance to heat flow across the interface of two materials. It arises due to differences in acoustic and thermal properties between the materials. When two materials with different phonon spectra meet, phonon scattering occurs, impeding heat transfer and increasing ITR. High ITR can lead to inefficient heat transfer and overheating, posing significant challenges for thermal management in electronic devices.[1]

Conversely, high ITR interfaces are crucial for applications requiring thermal insulation. High ITR can be beneficial in decreasing heat loss, increasing the efficiency of thin-film thermoelectrics, maintaining stable working conditions for sensors, and serving as thermal insulating layers for phase change memory—a promising non-volatile storage technology.[2,3]

Several models exist to predict ITR, including the Acoustic mismatch model (AMM) and the Diffuse mismatch model (DMM).[4] The AMM assumes that phonons behave like waves and are partially transmitted and partially reflected at the interface. The DMM, on the other hand, assumes that phonons are scattered diffusely at the interface, with the probability of transmission depending on the density of states and group velocities of the materials involved. Molecular dynamics (MD) is also commonly used to predict ITR. However, the simulation time and particle numbers are restricted to allow the full quantum calculation of the electronic structure for every configuration of atoms.

Additionally, all trajectories of the system often require more information than is known, limiting the accuracy and applicability of MD simulations.

Recently, machine learning models have shown promise in improving the accuracy of ITR predictions.[5] These models can leverage large datasets to identify patterns and correlations that traditional models might miss, such as the roughness of the interface, defects or impurities, film thickness, the presence of interfacial layers, and the adhesion between the materials. For instance, machine learning models can predict suitable material combinations for specific needs, such as high ITR interfaces for thermal insulation. By training on experimental data, these models can suggest the best material combinations with high ITR, such as using superlattices to achieve ultra-low thermal conductivity, which can be even lower than that of the corresponding amorphous counterparts, for effective thermal insulation.[6,7]

The accuracy of machine learning models heavily depends on the quality of the data they are trained on. High-quality, comprehensive databases are crucial for developing reliable predictive models. However, current databases often suffer from limitations such as incomplete data, measurement inconsistencies, and lack of standardization. Additionally, the data distribution is usually unbalanced. Most of the data focuses on metal/nonmetal interfaces because thermal measurement techniques often use metal as a heat transducer in the laser absorption and detection processes of the thermoreflectance technique (pump–probe method). Some interfaces have significantly more data points but also show considerable deviations due to different experimental synthesis conditions. Additionally, the heat transport mechanisms and primary carriers in metal/metal interfaces or two-dimensional (2D) materials are distinct from those in metal/nonmetal interfaces. As a result, these unique data may need to be carefully managed in the training datasets for ITR prediction models.[8]

Enhancing the quality and breadth of data available in these databases is essential for improving the performance of machine learning models in predicting ITR. Furthermore, the adoption of standardized protocols for data collection and reporting will ensure consistency and reliability across different studies and databases.

Inorganic, Amorphous, and 2D Materials in Thermal Management

Inorganic materials like silicon and various metal oxides are widely used in electronic devices due to their favorable electrical properties. Thin films of these materials, when used in layers or coatings, can significantly influence the thermal management of devices. For example, silicon dioxide (SiO_2) thin films are commonly used as thermal insulating layers in phase change memory.

Amorphous materials have emerged as key materials in integrated electronics, energy storage, and data applications. Their properties, including the absence of grain boundaries found in polycrystals, make them appealing for preventing leakage effects. Despite their potential, their thermal properties can be less predictable compared to crystalline materials, necessitating detailed studies to understand and optimize their behavior in specific applications.

Two-dimensional (2D) materials, such as graphene and transition metal dichalcogenides (TMDs), have shown remarkable potential in improving thermal management in electronics. These materials possess anisotropic thermal properties[9] due to their atomic thickness and high surface area-to-volume ratio. For instance, graphene, with its high thermal conductivity, can effectively spread heat and reduce localized hot spots in electronic devices. TMDs, on the other hand, offer tunable thermal properties through various structural modifications, making them suitable for tailored thermal management solutions. Incorporating 2D materials into existing interfaces can further optimize ITR and enhance overall device performance[10], building on the advances made with inorganic and amorphous materials. This integration highlights the potential for significant improvements in thermal management through the combined use of various advanced materials.

Innovative Approaches in Material Design

One innovative approach in material design is the use of composite materials, which combine the best properties of different materials to achieve superior thermal performance. For instance, incorporating high thermal conductivity materials like graphene or carbon nanotubes into a matrix can create composites with excellent thermal management capabilities.

Nanostructuring is another promising technique for improving interfacial heat transport. By engineering materials at the nanoscale, we can create structures that facilitate efficient phonon transport for targeted applications. Machine learning can significantly enhance nanostructuring in two ways: selecting the optimal materials for the interfaces and optimizing the structure, such as choosing between periodic or aperiodic superlattices. By predicting the ITR of various configurations, we can identify the most promising candidates for experimental validation, thereby accelerating the development process. Additionally, Bayesian optimization can efficiently design structures for applications requiring spectral-selective thermal radiation, such as thermal radiators and thermal radiative cooling.[11,12]

Thermoelectric devices,[13] which convert heat into electricity, also benefit from optimized interfacial heat transport. By selecting optimal interfaces with high ITR and optimizing their layered structures to achieve low thermal conductivity, thermoelectric devices can increase their conversion efficiencies, making them more viable for applications in waste heat recovery and renewable energy.

Another area of application is in energy storage devices, such as batteries and supercapacitors. Thermal management in these devices is crucial to ensure safe operation and prevent thermal runaway, which can lead to catastrophic failures. Optimized interfacial heat transport can help maintain uniform temperature distribution, enhancing the safety and performance of these energy storage systems.

Future Research Directions

Future research should focus on improving database quality and integrating advanced models for predicting ITR. This includes expanding existing databases to encompass high-quality, comprehensive data and standardizing datasets to ensure consistency and reliability. Additionally, developing hybrid models that combine traditional approaches with machine learning can enhance the accuracy and reliability of ITR predictions.

Exploring new materials and nanostructures for better thermal management is another promising direction. By leveraging the capabilities of machine learning and advanced modeling techniques, we can design materials with tailored thermal properties that meet the specific needs of next-generation electronic devices.

Interfacial heat transport is a critical aspect of thermal management in electronics. Advances in modeling and material design, supported by high-quality data, are essential for addressing the challenges in this field. Combining machine learning with traditional approaches will drive innovation, leading to next-generation electronic devices with superior thermal performance, reliability, and efficiency in an increasingly demanding technological landscape.

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