Interfacial thermal management of inorganic thin films from predictions to applications via materials informatics

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Interfacial heat transfer plays a crucial role in materials design and device performance. High interfacial thermal resistances (ITRs) affect the device efficiency and increase the energy consumption. On the contrary, high ITRs can enhance the figure of merit of thermoelectric materials by achieving ultra-low thermal conductivity via nanostructuring. Lots of factors affect ITRs making ITRs prediction a high-dimensional mathematical problem. We proposed an unprecedented ITRs predictive model considering the physical, chemical, and material properties to address it. Those descriptors assist the models in reducing the mismatch between predicted and experimental values and reaching high predictive performance of 96%, which is much higher than the common-used acoustic mismatch model (AMM) and diffuse mismatch model (DMM) of 60%. Here, two examples of the interfacial thermal management via materials informatics will be demonstrated: the Bi/Si composite thin films for thermal insulators and Au/MoS_2 monolayer for high efficient 2D-material electronic devices. The former is selected from the ITRs predictive model and achieve an ultra-low thermal conductivity of 0.16 $Wm^{-1}K^{-1}$ among porous-free composite thin films. The ultralow thermal conductivity is attributed to the high Bi/Si interfacial area by nanostructuring via combinatorial sputtering. The latter is an improvement of thermal transport at Au/MoS_2 monolayer interfaces by tuning the interfacial chemical condition. The ITRs database clearly shows the interlayer effect such as oxygen plasma treatment at interface on the ITRs, leading to the findings that adequate oxygen adsorbates at the Au/MoS_2 interface improve the thermal and electrical conductance, in agreement with the DFT simulated results. By means of the broad exploration of materials informatics (machine learning), the hints from the database and prediction could accelerate the materials development. More details and further undiscovered issues will also be discussed in the talk.