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Molecular dynamics simulation of the thermal transport across Si/Al interfaces WOON IH CHOI, KWISEON KIM, SREEKANT NARUMANCHI, NREL — Efficient heat dissipation is critical for power electronics where the device package consists of several layers of different materials. Conventional thermal interface materials are bottlenecks in heat removal. Detailed understanding of interfacial heat resistance would benefit efforts to improve the device design. We have chosen Si/Al interfaces for this thermal transport study. We construct Si-Al MEAM interatomic potential parameters based on the density functional theory (DFT) calculations. We generate various interface structures using the first-principles molecular dynamics (MD) simulations. Using the direct method to compute the thermal conductance, we investigated various interface structures. We will discuss the effect of the inter-diffused layers and roughness of the interfaces on the thermal boundary conductance. We will also compare our result with limited data in the literature.

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