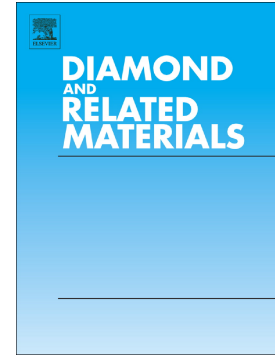


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**Theoretical modelling for interface design and thermal conductivity prediction in
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Abstract

Interface design is essential for diamond/Cu (Dia/Cu) composites to achieve high thermal conductivity (TC), due to the incompatibility between diamond particles and Cu matrix. In this work, a physical model was developed to theoretically reveal the effects of different interface layers on the TC of Dia/Cu composites. The results indicate that the thickness, intrinsic TC, phonon velocity and carbide transformation of interface layers and their solubility in Cu matrix greatly affect the thermal performance of the composites. Interface layers with nanoscale thickness (e.g. smaller than 200 nm) are desirable to improve the TC of Dia/Cu. The carbide transformation affects the TC differently via varying the phonon mismatch between Dia/Cu and thermal resistance of interface layers. W-WC layer is the most favorable candidate to achieve high thermal performance, which agrees well with experimental results. This study supplies an overall but specific consideration for the interface design in Dia/Cu composites for the first time, and offers a fundamental guide for experiments of interface modification, which is also applicable for other matrix composites.

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