Thermal Conductivity of Composites: How Comsol Revealed an Omission in a Classical Paper

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Abstract

The initial motivation for this work was to explore the relationship between the shape of particles and the thermal conductivity of nanofluids or nanocomposites containing them. Since the possibility for manufacturing exotically-shaped particles is ever growing, it was thought useful to devise a way to select which materials and shapes have a potential for better thermal properties.

Literature [1] suggests that a wide range of experimental data on nanofluids can be well represented by a standard conduction model taking into account an interfacial resistance between the particles and the matrix in which they are embedded. In practice, the heat conduction problem is solved in a cubic cell containing one particle and submitted to a unit temperature gradient on two opposite sides and a zero-flux condition on the others. The heat flux through the cell is computed and translated into an equivalent conductivity K. The calculation is repeated for various particle sizes, corresponding to various particle volume fractions v. The K-v relationship is then analyzed as a series expansion K/Km = 1 + [K].v + O(v2) where Km is the conductivity of the matrix and [K], termed the "intrinsic conductivity", is the final result. The computations were done using COMSOL Multiphysics with two "Heat Transfer in Solids" interfaces coupled by a flux condition. An "extra-fine" physics-controlled meshed was used in most cases.

For the sake of validation, this procedure was applied to the case of spherical or ellipsoidal particles that is treated analytically in a classical 1997 paper by Nan et al. [2]. Excellent results were obtained with particles without interfacial resistance, as shown on Figure 1 (Kp: conductivity of the particles; // and perp: parallel and perpendicular to the axis of revolution of the ellipsoids; p is the aspect ratio; dashed lines: ±2%). On the other hand, agreement was very poor when interfacial resistance was introduced (Figure 2), in spite of attempts at global or local mesh refinement, change of solver or use of approximate models in the case of high Kp/Km ratios.

In the face of these repeated failures, it was thought that the problem might stem from the analytical equations and decided to go back to their derivation in the original paper. The latter calculates the contribution of the interfacial layer by embedding the ellipsoidal particle in a constant-thickness layer that is made vanishingly small. Careful scrutiny of the derivation showed that two erroneous assumptions had been made in [2]: firstly, the external layer was assimilated to an ellipsoid; secondly, it was assumed to have the same aspect ratio as the particle. Taking the first point into account proved far beyond the mathematical skills of the author. On the other hand, it was possible to modify Nan et al.'s formulae for the aspect ratio effect and to obtain a much

improved (though not perfect) agreement as shown by Figure 3 (dashed lines: ±10%).

Reference

1. J. Buongiorno et al., A benchmark study on the thermal conductivity of nanofluids, Journal of Applied Physics, 106, 9, 094312-1-094312-14 (2009)

2. C.W. Nan et al., Effective thermal conductivity of particulate composites with interfacial thermal resistance, Journal of Applied Physics, 81, 10, 6692-6699 (1997)