Topology Optimization of Nanoscale Heat Conduction with the Boltzmann Transport Equation

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Abstract

Thermoelectric devices are devices that allow direct conversion between thermal and electric energy. That is, a voltage is generated when there is a temperature gradient between two different points on the device, and, conversely, given a voltage difference between two different points, a temperature gradient is generated. The miniaturization of thermoelectric devices has driven the need to improve the heat conduction performance in these devices. In our research, we focus on the level set-based topology optimization of heat conduction at the nanoscale, to obtain improved designs for thermoelectric devices.

Macroscale and nanoscale heat conduction phenomena are quite different. According to Fourier's law, which is used when analyzing macroscale heat conduction, heat flux is proportional to the temperature gradient of a system and the heat conduction is an isotropic conduction. On the other hand, nanoscale heat conduction is ballistic, and analysis of this type of heat conduction is required to obtain improved designs for thermoelectric devices that depend on nanoscale phenomena. In 1993, A. A. Joshi and A. Majumder pioneered the use of the Boltzmann transport equation to numerically analyze nanoscale heat conduction. However, until now, high performance thermoelectric devices have been designed through trial and error, and research on design methods for constructing thermoelectric devices focused on nanoscale behavior has been scarce.

Topology optimization, which can dramatically change both structural shape profiles and the number of holes in a structure during optimization procedures, is widely used in many structural design problems. A level set-based topology optimization method, proposed by Yamada et al [1], has been applied to a variety of optimization problems involving different physical phenomena. In this design method, the iso-surface of a scalar function, the level set function, represents structural boundaries and structural profiles are optimized by updating the level set function, based on design sensitivity information. This method therefore always provides optimal configurations that have clear boundaries. When dealing with design problems at the nanoscale, scattering effects and the penetration of phonons at the material boundaries must be considered. We extend a level set-based topology optimization method to enable accurate analysis of nanoscale heat conduction in a structural design problem. For this extension, we derive the topological derivative as the design sensitivity. This derivative can precisely evaluate differences in the value of the objective functional when a hole is generated, i.e., when a new boundary is generated, during the optimization procedure. In this manner, we obtain optimal configurations that include consideration of scattering effects and the penetration of phonons, based on the topological derivative.

In this work, we present the following four items: (1) design requirements and an objective functional for the optimization problems; (2) derivation of the topological derivative as the design sensitivity; (3) development of the optimization algorithm for the design problem; and (4) numerical examples of topology optimization for a thin film structure of a thermoelectric device, to confirm the effectiveness and utility of the proposed method.

Keywords: Topology Optimization, Boltzmann Transport Equation, Nanoscale Heat Conduction

References

[1] Yamada, Takayuki, et al. "A topology optimization method based on the level set method incorporating a fictitious interface energy." *Computer Methods in Applied Mechanics and Engineering* 199.45 (2010): 2876-2891.