MATERIALS ENGINEERING SEMINAR

"Thermal Transport in Irradiated Thorium Dioxide"

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Purdue MSE Ph.D. Final Exam

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ABSTRACT

The current research focuses on predictive modeling of phonon-mediated thermal transport in thorium dioxide (ThO_2) with defects. ThO_2 has lately gained attention as a model material for fundamental investigations of thermal transport degradation under irradiation, which is relevant to fuel performance in nuclear reactors. Thermal transport in irradiated ThO_2 is first modeled here by a non-transport solution of the linearized Boltzmann transport equation (BTE) within the single-mode relaxation time approximation. Classic models for phonon-defect scattering rates are used to model point defects, voids, and dislocation loops in irradiated ThO_2 and the resultant thermal conductivity is directly compared to experimental measurements of irradiated specimens. Our predicted conductivity values agree well with measured values near room temperature. However, discrepancy between our predictions and experimental values exist at lower temperatures where experimentally measured conductivity values seem to reach a saturation level while the model predicts further reduction in thermal conductivity. This discrepancy is most notable in higher irradiation dose samples where the thermal conductivity is almost completely controlled by the dislocation loop density. This hints at the conclusion that classic models for phonon-defect scattering rates which integrate out local variation of the defect strain field and replace this by a defect density may not be adequate to capture all physics of phonon-defect scattering, especially for dislocation loops at low temperatures. This motivated us to model defects through their spatially resolved lattice distortion fields and explicitly investigate phonon scattering in those fields in an explicit fashion. A transport solution of the phonon BTE is implemented based upon the Monte Carlo (MC) method, which explicitly tracks the phonon population as it evolves in space and time according to phonon group velocities and scattering rates. An expression for the scattering rate of phonons from an arbitrary strain field is derived from a generalized form of Grüneisen's law of thermal expansion, and applied to the case of dislocations in ThO_2. It is found that the localized strain in the material, resulting from the presence of a crystal defect, leads to a net heat flux into the strained region. This provides evidence for thermal fluxes in the absence of a temperature gradient, a phenomenon that cannot be captured via Fourier's law. Although the model is applied specifically to the case of dislocations in ThO_2, the derived phonon scattering rate expression is general and may be applied to any defect for which a strain field may be generated.

Date: Monday, June 19, 2023
Time: 10:00 A.M.
Place: ARMS 1021 or via Zoom: https://purdue-edu.zoom.us/j/5211402390

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