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Lattice Thermal Conductivity in ε-Ga_2O_3 MICHAEL MEHL, Physics Department, US Naval Academy, Annapolis MD, N. NEEPA, V. D. WHEELER, D. J. MEYER, Electronic Science and Technology Division, US Naval Research Laboratory, Washington DC — β-Ga_2O_3 has seen increased popularity as a substrate and device material because of its large band gap and theoretical breakdown field, but it suffers from low thermal conductivity (κ). The question arises whether other polytypes of Ga_2O_3 might have higher thermal conductivity along with an ultra-wide band gap. One potential phase is is ε-Ga_2O_3, which has a large band gap (4.9 eV) and a wurtzite-like crystal structure. Unfortunately, the ε phase is difficult to model from first principles, as several of the Ga Wyckoff positions are only partially occupied. In this talk we examine several structures which approximate ε-Ga_2O_3. For these structures we then calculate the lattice contribution to the bulk thermal conductivity tensor κ by computing second- and third-order force constants. We compare our results with experimental and theoretical data for β-Ga_2O_3.

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