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Revisiting the theory of disordered alloy thermal conductivity HAMID REZA SEYF, LUKE YATES, THOMAS BOUGHER, SAMUEL GRAHAM, BARATUNDE COLA, THEERADETCH DETCHPROHM, MI-HEE JI, JEOMOH KIM, RUSSELL DUPUIS, WEI LV, ASEGUN HENRY, Georgia Institute of Technology, RUSSELS' GROUP COLLABORATION, NANO ENGINEERED SYSTEMS AND TRANSPORT LAB COLLABORATION, ELECTRONICS MANUFACTURING AND RELIABILITY LABORATORY COLLABORATION, THE ATOMISTIC SIMULATION & ENERGY (ASE) RESEARCH GROUP COLLABORATION — Current understanding of the phonon contributions to alloy thermal conductivity (TC) is based on the phonon gas model (PGM) and the virtual crystal approximation (VCA). Using this theoretical framework, good agreement is obtained in some cases, but there are many instances where it fails – both quantitatively and qualitatively. Here, we reexamine the conventional theory and note that a critical assumption is that all of the phonons/normal modes of vibration resemble plane waves with well-defined velocities. Instead, we show that in a random alloy, the character of the normal modes changes dramatically within the first 2% impurity concentration, beyond which they more closely resemble the modes found in amorphous materials. We then utilize a new theory that can treat modes with any character and experimentally confirm its new insights. The results indicate that mode character is critical and has significant implications for phonon interactions with neutrons, electrons and photons, since the momentum of non-propagating phonons is currently unknown.

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