Thermal transport by extended and localized phonons in mixed cryocrystals.

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As a crystal becomes increasingly more disordered, a point may be reached, where the typical phonon mean-free path becomes so short that the wavelength and mean-free path are no longer a sharp concept, and the phonon gas model for thermal conductivity breaks down. The most successful alternative models hypothesize that the phonons are weakly localized by the disorder structure and diffuse among the neighboring localization sites by a random walk [1-2] or through the hopping process [3-4]. The concept of minimum thermal conductivity [1-2] is based on the picture were the lower limit to the conductivity is reached when the heat is transported through a random walk of the thermal energy between the localized quantum mechanical oscillators. The lifetime of each oscillator is assumed to be one half the period of vibration. This model predicts that the thermal conductivity coefficient will become temperature-independent at a sufficiently high temperature. In the thermally activated hopping (TAH) model the thermal conductivity coefficient will be proportional to T at high temperatures.

To compare correctly experimental results of thermal conductivity with theory at high temperatures, it is necessary to perform experiments at a constant density to exclude the effect of thermal expansion. In this study the isochoric thermal conductivity of the $Kr_{1-\xi}Xe_{\xi}$ and $Kr_{1-\xi}(CH_4)_{\xi}$ solid solutions ($1\geq\xi\geq0$) was measured in a wide range of concentrations at $T\geq\Theta_D$ (Θ_D is the Debye temperature). As ξ increases ($0.5\geq\xi\geq0$), the thermal conductivity decreases as a hole and increases less steeply with decreasing temperature. In the middle of the composition range the thermal conductivity was temperature-independent and its absolute value was in good agreement with lower limit to thermal conductivity Λ_{min}, calculated according to [2]. The quantitative description is given in the framework of the Debye model of thermal conductivity that contains extended phonons and localized phonons above a mobility edge. The localized phonons carry heat through a random walk of thermal energy. In pure Kr the thermal conductivity is of pure extended-phonon character up to about 90 K. As the impurity concentration increases, progressively more heat is transported by the localized phonons. The contribution of extended phonons to the total thermal conductivity is about 10% in the middle of the composition range.

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