

Structure–property relationships in Fe–Ge intermetallics: Spotlight on Nowotny Chimney Ladders

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The crystal structure of a material fundamentally dictates its electronic and thermal transport properties, making it a critical factor in determining thermoelectric performance [1]. This research explores this profound influence by focusing on three distinct FeGe, Fe₂Ge₃, and FeGe₂ phases in the Fe–Ge system [2]. Despite being built from iron and germanium atoms, these compounds exhibit unique stoichiometric ratios and, crucially, possess vastly different crystal structures. This structural diversity is hypothesized to significantly alter their electronic band structures and phonon scattering mechanisms, which are fundamental to efficient thermoelectric energy conversion.

A particular emphasis is placed on the Nowotny Chimney Ladder (NCL) Fe₂Ge₃ phase. The obtained results reveal that NCL Fe₂Ge₃ exhibits a significantly enhanced Seebeck coefficient of up to $-165.4 \mu\text{VK}^{-1}$ compared to approximately $10 \mu\text{VK}^{-1}$ for FeGe and $-3 \mu\text{VK}^{-1}$ for FeGe₂, leading to a higher power factor of $14.3 \mu\text{Wcm}^{-1}\text{K}^{-2}$. Furthermore, its unique crystal structure contributes to remarkably lower lattice thermal conductivity $1.6 \text{Wm}^{-1}\text{K}^{-1}$ at room temperature relative to its counterparts (FeGe $2.9 \text{Wm}^{-1}\text{K}^{-1}$ and FeGe₂ around $4.2 \text{Wm}^{-1}\text{K}^{-1}$). This combination of enhanced electronic and disturbed thermal transport results in NCL Fe₂Ge₃ demonstrate the highest thermoelectric figure of merit (*ZT*) among all three phases at relevant temperatures, achieving a peak *ZT* of 0.43 at 623 K. By meticulously correlating the individual crystal structure of FeGe, NCL Fe₂Ge₃, and FeGe₂ with their measured and calculated transport parameters, we demonstrate that crystal structure profoundly impacts charge carrier dynamics and phonon scattering. Our results confirm that crystal structure engineering is a powerful strategy for optimizing high-performance thermoelectric materials, with NCL Fe₂Ge₃ serving as a compelling example for future material design.

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