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# Phonons in the filled skutterudites under high pressure studied by nuclear inelastic scattering

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The word's demand of the sustainable energy and efficient heat-to-energy conversion brings high interest to the thermoelectric materials. Between all new materials one of the promising classes is the structures containing empty voids filled by loosely bound "rattling"atoms, like skutterudites and clathrates which strongly scatter the propagating acoustic phonons thus decreasing the thermal conductivity. Even after 20 years of the intensive study the microscopic mechanism of the suppression of the thermal conductivity is unclear and highly debated. The original idea of the non-correlated, independent of the host structure, vibrations of the "rattling"atoms [1] has been contested by the inelastic neutron and nuclear inelastic measurements [2,3]. At the same time, purely harmonic Einstein oscillation of the "rattling"atoms cannot explain the reduced thermal conductivity. Thus, the strongly anharmonic interatomic potential of the "rattling"atoms and the hybridization of the "rattling"optic mode and acoustic propagation mode were suggested as a possible origin of the thermal conductivity suppression [4].
Here, we report [5] on study of the lattice dynamics in the filled skutterudite EuFe4Sb12 by nuclear inelastic scattering, a technique which through its element selectivity provides partial densities of phonon states individually for all three elements presented in the compound. This allows us to compare vibrations of the guest atoms and of the host structure. In order to study the anharmonicity of the vibrations the system was investigated under high pressure in combination with the powder X-ray diffraction. As result the element specific Grüneisen parameters were obtained for a set of individual phonon modes. A large Grüneisen parameter was found for the "rattling" mode which is hybridized with the acoustical phonons at ambient and moderate pressure. However, at critical pressure of 12 GPa the Grüneisen parameter for the "rattling" mode is reduced and phonon modes decouple. The results of this study are important for understanding of the microscopic mechanism of the lattice dynamics in the guest-host structures like filled skutterudites.

References

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