Skutterudites: An Update

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Materials with the skutterudite crystal structure possess attractive transport properties and have a good potential for achieving ZT values substantially larger than for state-of-the-art thermoelectric materials. Studies conducted at JPL on $CoAs_3$, $RhAs_3$, $CoSb_3$, $RhSb_3$ and $IrSb_3$ have shown that p-type conductivity samples are characterized by carriers with low effective masses and very high nobilities, low electrical resistivities and moderate Seebeck coefficients. The carrier nobilities of n-type samples are about an order of magnitude lower, but low electrical resistivities and relatively large Seebeck coefficients can still be obtained at high doping levels. The room temperature lattice thermal conductivities of these binary skutterudites was found to be 7 to 10 times larger than that of Bi_2Te_3. This results in low ZT values at 300K, though heavily doped n-type $CoSb_3$ samples can achieve $ZT \sim 1$ at 600°C.
Several research groups, mostly in the U. S., are now working on understanding and optimizing the transport properties of skutterudites. Most of the efforts are focusing on reducing the lattice thermal conductivity by filling the empty octant cages in the skutterudite structure with rare earth atoms. Additional approaches have also been pursued at JPL, in particular the formation of solid solutions and alloys, and the study of novel ternary skutterudite compounds. Recent experiments have demonstrated that ternary compounds such as $Ru_{0.5}Pd_{0.5}Sb_3$ and filled skutterudites such as $CeFe_4Sb_{12}$ had much lower lattice thermal conductivity. High ZT values have been obtained for several filled skutterudites in the 500-700°C temperature range, but figures of merit at 300K are still low. This paper reviews recent experimental and theoretical results on skutterudites with a particular emphasis on the transport properties of ternary compounds and filled compositions. The latest results obtained at JPL are presented and the possibility of obtaining high ZT values near room temperature is discussed.

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