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Rare-earth-based half-Heusler compounds as prospective materials for thermoelectric applications

D. Kaczorowski[1], K. Gofryk[1], A. Leithe-Jasper[2], Yu. Grin[2]

[1] *Institute of Low Temperature and Structure Research, Polish Academy of Sciences, P.O. Box 1410, 50-950 Wrocşaw, Poland*

[2] *Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany*

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Heusler phases of the general compositions XYZ and XY_2Z, where X and Y stand for d- or f- transition metals and Z denotes a p-element, continuously attract much attention because of a large variety of their interesting physical properties. With respect to the character of electrical conductance they range from good metals to wide-gap semiconductors. Magnetically they may behave like diamagnets or weakly-temperature-dependent paramagnets but they may also show Curie-Weiss paramagnetism. Frequently these materials exhibit long-range magnetic ordering that may have itinerant character but it may show a well localized nature as well. Last but not least some Heusler phases exhibit unusual properties characteristic of strong electronic correlations. Due to all these features Heusler-type compounds are being intensively studied in the context of plenitude of topics, e.g. metal-insulator transition, Kondo effect, heavy fermions, superconductivity, giant magnetoresistance, half-metals, semimetals, magnetic semiconductors, shape-memory alloys, etc. In half-Heusler alloys XYZ the presence of vacancies often leads to the formation of a narrow gap in the density of electronic states near the Fermi level. Owing to that these compounds usually exhibit large magnitudes of the thermoelectric power, which together with their relatively low electrical resistivity and thermal conductivity make them promising materials for thermoelectric applications. In the course of our systematic investigations of $4f$-electron based Heusler compounds, the physical properties of two series of XYZ phases with the composition REPdSb and REPdBi (RE = Y, Nd, Gd, Dy, Ho, Er) have recently been studied by means of magnetization, magnetic susceptibility, electrical resistivity, magnetoresistivity, thermoelectric power and Hall effect measurements, performed in the temperature range 1.5–300 K and in magnetic fields up to 12 T. All these ternaries, but diamagnetic YPdSb and YPdBi, exhibit localized magnetism of RE^{3+} ions. The compounds DyPdSb, HoPdSb, NdPdBi, GdPdBi, DyPdBi and HoPdBi order antiferromagnetically at low temperatures (T_N = 2–13 K), whereas ErPdSb and ErPdBi remain paramagnetic down to 1.5 K. Both series show half-metallic conductivity, presumably due to the presence of narrow gaps of the order of tens meV in the electronic band structures near E_F. All these ternaries show very high values of the Seebeck coefficient at room temperature (S up to 200 μV/K), characteristic of semimetals. The carrier concentrations estimated from the Hall data are of the order of 10^{19}–10^{20}/cm^3. The measured thermal conductivities are rather low being few W/mK at 300 K. As a result, the thermoelectric figure of merit reaches values of about 0.2 at room temperature, i.e. ZT is similar to those found for doped 3δ-electron transition metal based XYZ phases and "rattling" systems like skutterudites and clathrates, which are currently intensively investigated in a field of possible applications as novel thermoelectrics. Furthermore, the heat conductivity in the REPdSb and REPdBi compounds is dominated by the phonon contributions, and hence it should be possible to improve their thermoelectrical performance by means of controlled doping (alloying) of the host lattice or/and by increasing the level of structural disorder by appropriate heat treatment.