Supplementary Material

Properties of HPT-processed large bulks of p-type skutterudite $DD_{0.7}Fe_3CoSb_{12}$ with high ZT > 1.3

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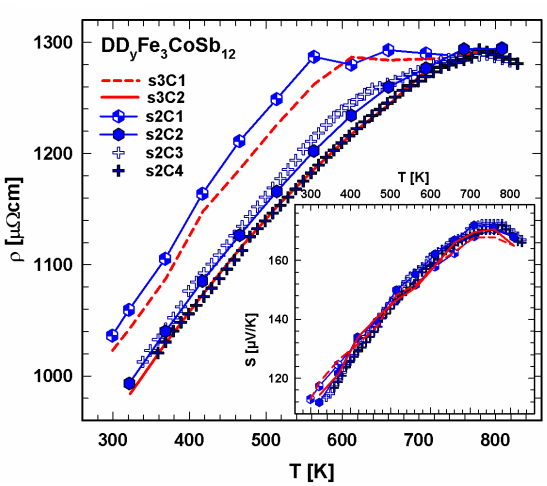

Fig. S1. $DD_yFe_3CoSb_{12}$: electrical resistivity, ρ, vs. temperature, T, of samples s2 and s3. Insert: Seebeck coefficient, S, vs. temperature T.

Figure S1 demonstrates that the temperature-dependent electrical resistivity and the Seebeck coefficient (Insert in Fig. S1) of samples s2 and s3 exhibit, within the error bar, the same values, thus making it possible to combine results of specimens of both samples. In addition,

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one can see that a second measurement with in- and decreasing temperature (s2C3 and s2C4 in Fig. S1), performed with a different equipment in a different lab, confirms not only thermal stability after the first run, but also the accuracy of the original measurement.

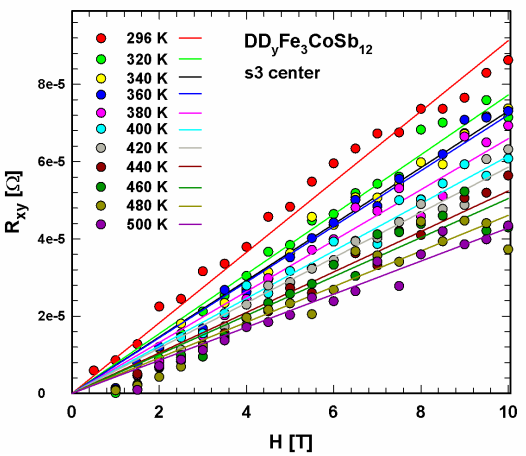

Fig. S2. $DD_yFe_3CoSb_{12}$: Hall resistivity, R_{xy}, vs. magnetic field, H, with least squares fits according to $R_{xy} = k_H.H$.

Exemplarily shown in Fig. S2 is the isothermal field dependent Hall resistance R_{xy} for various temperatures of the sample s3-center. The almost linear dependence of $R_{xy}(H)$ enables the application of the classical single band model, and the positive Hall resistance refers to holes as dominating charge carriers. In this scope, the charge carrier density n follows from

$$n = \frac{H}{q \,.\, R_{xy}} \,.\, \frac{1}{d_s} \,, \qquad \text{(S1)}$$

where q is the elementary charge, R_{xy} the Hall resistance at a finite value of the experimentally applied magnetic field H and d_s stands for the thickness of the measured sample. The Hall mobility μ can then be evaluated from

$$\mu = 1/\,(q\, n\, \rho_{xx}); \qquad \text{(S2)}$$

ρ_{xx} is the electrical resistivity, obtained at the same temperature as R_{xy}.

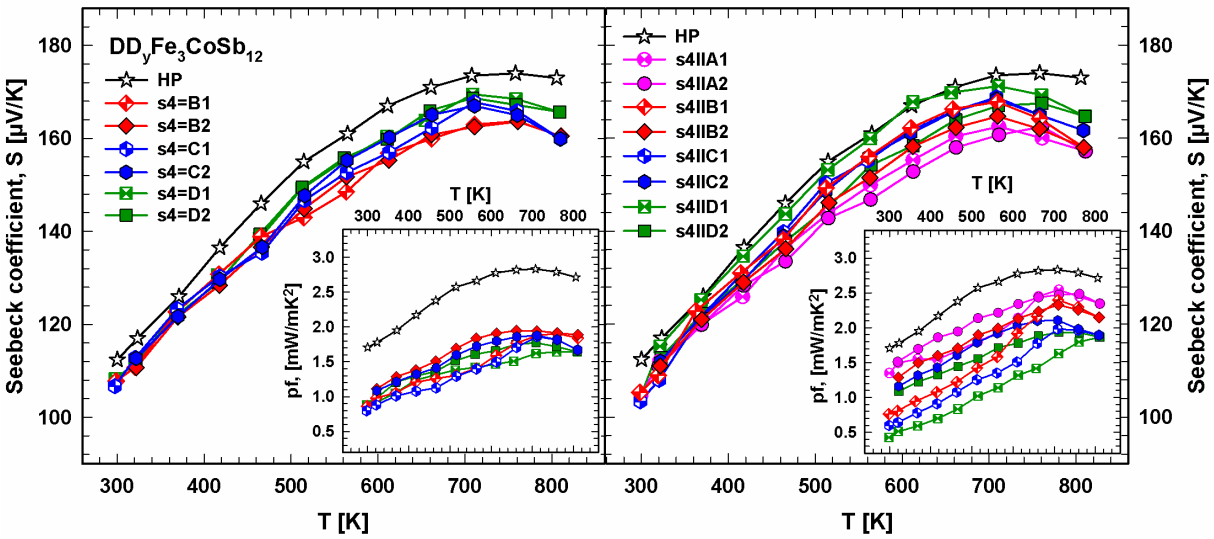

Fig. S3. $DD_yFe_3CoSb_{12}$: Seebeck coefficient, S(T), vs. temperature, T, of sample s4= (left panel) and of sample s4II (right panel). Insert: Temperature dependent power factor, pf.

Figure S3 shows that the Seebeck coefficient and power factor of sample s4= (left hand side) and of s4II (right hand side). As insert the power factor is displayed.

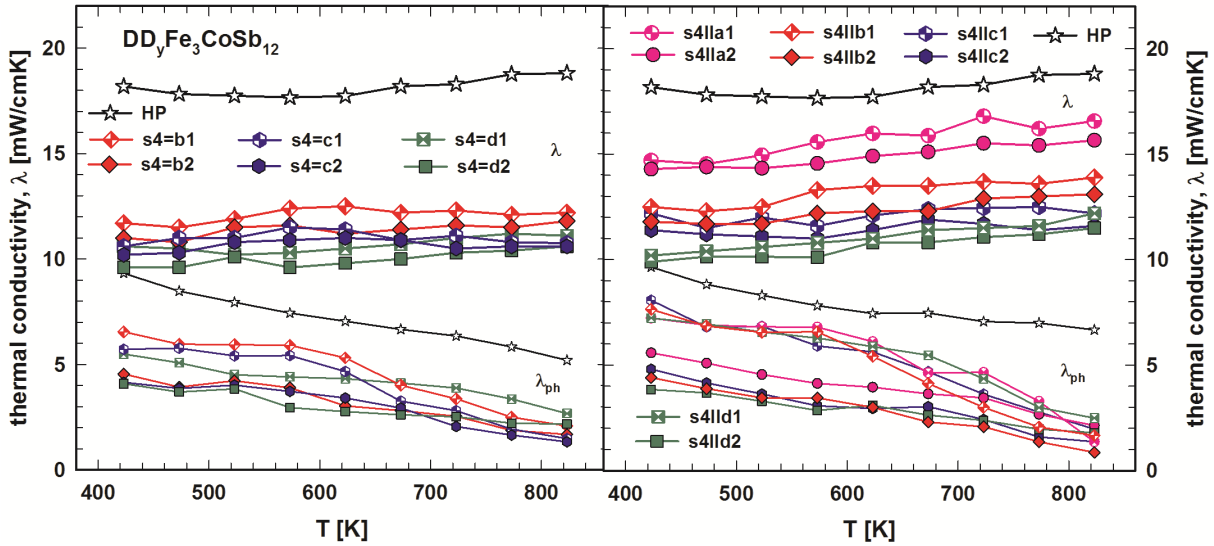

Fig. S4. $DD_yFe_3CoSb_{12}$: thermal conductivity, λ, and lattice thermal conductivity, λ_{ph}, vs. temperature, T, of sample s4= (left panel) and of sample s4II (right panel).

Figure S4 depicts the thermal conductivity and lattice thermal conductivity of sample s4= (left hand side) and s4II (right hand side). For specimens b, c and d the values are in the same range.

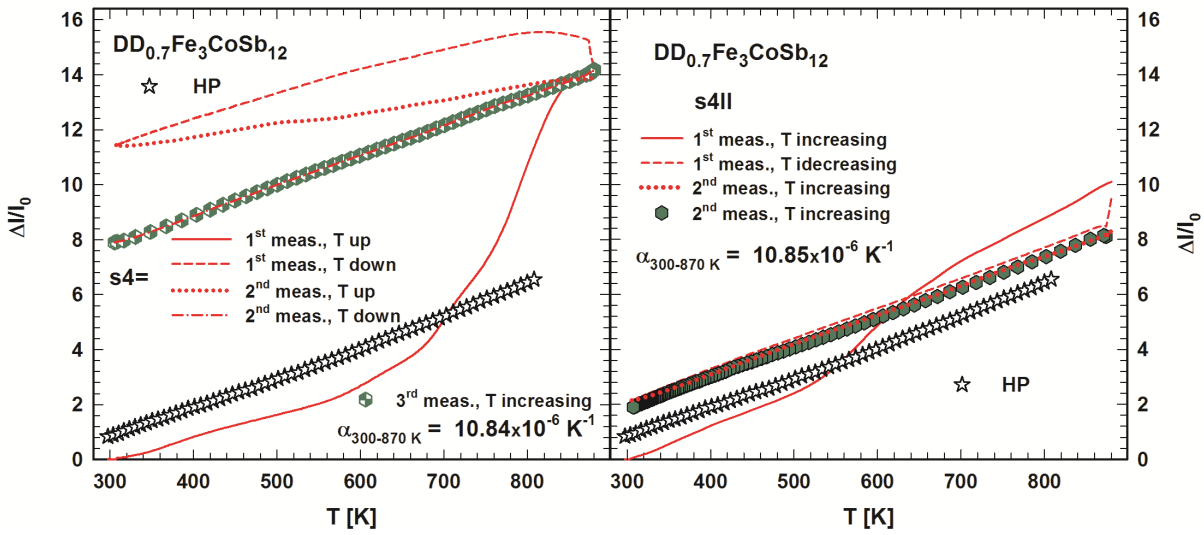

Fig. S5. $DD_{0.7}Fe_3CoSb_{12}$: thermal expansion, $\Delta\ell/\ell_0$ vs. temperature, T, for samples s4=(left) and s4II (right).

Fig. THEX. shows the thermal expansion of two specimens of sample s4 cut perpendicular to each other. For the first measurement with increasing temperature in both cases the temperature dependent $\Delta\ell/\ell_0$ curve runs till about 600 K parallel to the $\Delta\ell/\ell_0$ curve of the HP sample, indicating the same thermal expansion coefficient in this temperature region, followed by a steeper curve, which is different for s4= and s4II. Similar differences are obvious for ρ(T) during heating, but leading to the same ρ(T) for cooling. In case of thermal expansion after cycling twice (s4II) or three times (s4=) the $\Delta\ell/\ell_0$ curve becomes thermally stable, exhibiting practically the same average thermal expansion coefficient, $\alpha = 10.85 \times 10^{-6}$ K^{-1} and $\alpha = 10.84 \times 10^{-6}$ K^{-1}, respectively in the temperature range of 300-870 K.