Microstructure of advanced thermoelectrics after high pressure torsion

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Thermoelectrics (TE) are utilised for direct conversion of thermal energy into electrical energy and vice versa. Skutterudites are one group of thermoelectrics with promising parameters and they have already achieved fair efficiency for the conversion of heat to electricity. Researchers are trying to further enhance the figure of merit by various ways, e.g. nanostructuring and/or mechanical alloying [1-4]. Mechanical properties of the resulting materials are important as well. Theory shows that the only way how to increase the figure of merit of a thermoelectric material with optimized power factor is by shortening phonon free path and thus reducing thermal conductivity without changing electrical resistivity and Seebeck coefficient. This can be accomplished e.g. by enhancing the scattering of heat carrying phonons on lattice defects, impurities and grain boundaries. To introduce a high density of obstacles to phonon movement, various ways of severe plastic deformation can be used.

In this work we compare the microstructure of an industrial p-type $DD_yFe_3CoSb_{12}$ skutterudite processed by several routes. We started with a commercially produced skutterudite powder. It was further either (i) hot pressed (Ar atmosphere, 700°C, 56 MPa, 30 min, referred to as HP), or (ii) cold pressed (resulting in pellets 1 cm in diameter and about 1 mm in height, referred to as CP) followed by high pressure torsion (Ar atmosphere, 375°C, applying 4 GPa and 1 revolution, referred to as HPT), or (iii) ball milled (BM) followed by HP and HPT. Fracture surfaces of the processed samples were studied in a Tescan LYRA 3XMU SEM×FIB scanning electron microscope (SEM). Thin cross sectional lamellae were prepared by FIB (focused ion beam) in SEM. A Philips CM12 STEM transmission electron microscope (TEM) operating at 120kV and a JEOL JEM 2100F high resolution TEM operating at 200kV with an X-Max80 Oxford Instruments energy dispersive X-ray (EDX) analytical system were then used to study the microstructure. BM+HP+HPT route was selected as a regular way of preparation; CP+HPT represents a new energy and time saving route; HP sample was prepared as a reference. All samples reveal a bimodal grain size distribution (see an example for CP+HPT sample in Fig. 1), however with very different quantitative parameters. The average grain size decreases in the sequence HP > CP+HPT > BM+HP+HPT. Details of microstructure were studied by means of analytical TEM.

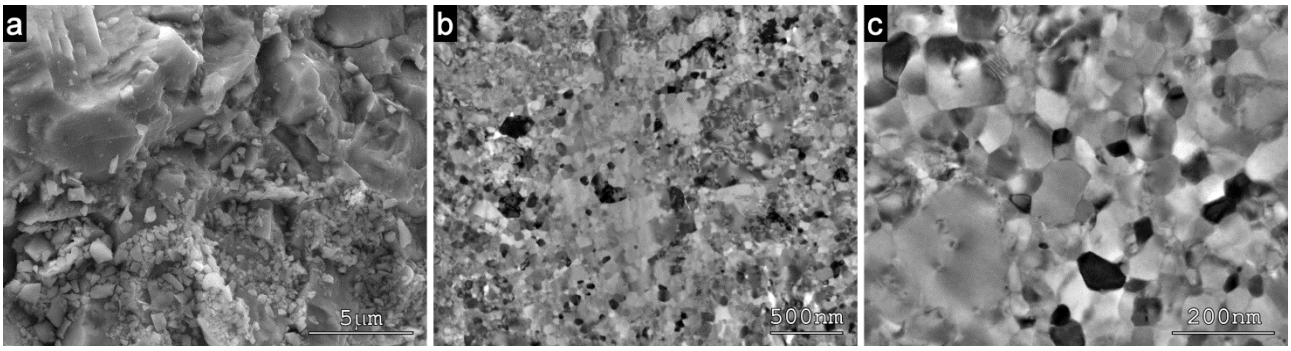

Figure 1. Sample CP+HPT: a SEM micrograph of fractured surface, image of secondary electrons (a) and TEM micrographs of thinned lamella (b, c).

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