Crystal structures of intermetallic Heusler compounds for spin-transfer torque applications and phase-separated half-Heusler compounds for thermoelectric applications

Juergen Winterlik, Teuta Gasi, Frederick Casper,Kai Filsinger, Olga Meshcheriakova, Michael Schwall, Benjamin Balke, Claudia Felser

Institut fuer Anorganische und Analytische Chemie, Johannes Gutenberg - Universitaet, 55099 Mainz, Germany.

Many important Heusler compounds and corresponding alloys contain elements with very similar atomic masses and hence similar scattering factors for ordinary XRD (Mn, Fe, Co, Ni, Ga). Anomalous XRD of these compounds and alloys for solving this problem by tuning the photon energy to the K-absorption edges of the corresponding elements.
In recent experiments we have determined the crystal structures of Fe-containing ferrimagnetic Heusler alloys (e.g. Mn_2FeGa, Fe_2MnGa). These compounds exhibit a peculiar tetragonal crystal structure which is impossible to determine using conventional Cu K_α powder XRD. Since the c/a ratio of these compounds is very close to 2 it was difficult to exclude a cubic structure for these compounds. Their hard-magnetic properties, however, pointed on a tetragonal distortion. Using anomalous XRD as depicted in Figure 1, recorded at beamline G3, we have verified the tetragonal structure and could exclude the cubic one due to the intensities of the reflections. We have furthermore found that the crystal structures exhibited large degrees of disorder, which requires further optimization of the technique of synthesis.

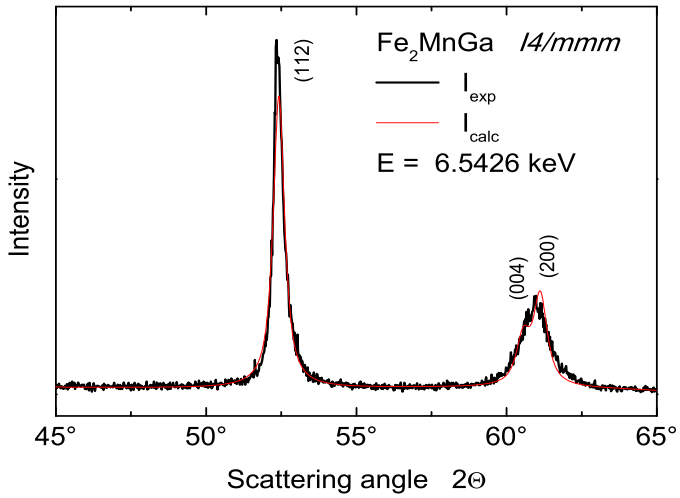

Figure 1: XRD pattern and fit of Fe_2MnGa at the Mn K-edge. The fit was performed assuming a structural model of space group I4/mmm ($a = 3.68$ Å, $c = 7.45$ Å) with random occupation of atoms on the different lattice sites. Evidently, the compound exhibits a high degree of disorder. Anyhow, the intensities and broadness of the (004) and (200) reflections clearly indicate that the structure is tetragonal or pseudocubic due to the c/a ratio close to 2.

Half-Heusler compounds offer highly useful prerequisites with respect to thermoelectric applications. In order to decrease the thermal conductivity to obtain higher figures of merit we have performed several successful experiments with the preparation of phase-separated Heusler compounds. The structures of these compounds required analysis with a very high resolution since the corresponding differences in the phase-separated structures are very small and could not be

resolved by conventional Cu K_α powder XRD. The diffraction pattern measured with Cu K_α synchrotron is shown in Figure 2. Evidently, the phase-separated structures are well resolved. The pattern was fitted by three Heusler phases with $C1_b$ structure (space group 216), which exhibit very similar lattice parameters. The determined lattice parameters of the three phases are a1=5.989 Å, a2=6.029 Å, and a3=6.075 Å. In comparison with the lattice parameter of the ternary compounds TiNiSn a=5.939 Å, ZrNiSn a=6.121 Åand HfNiSn a=6.091 Åit was possible to estimate the composition of the three phases qualitatively. The phase with the smallest lattice parameter a1=5.989 Åis very similar to TiNiSn and hints on a Ti-rich phase. The phase with the largest lattice parameter a3=6.075 Åseems to be a Hf-rich phase because of the very similar lattice parameter of HfNiSn.

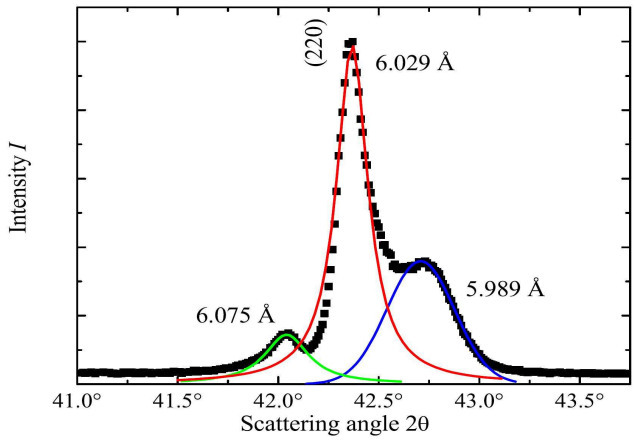

Figure 2: (220) reflection measured by synchrotron radiation.

Publications of these results are currently are currently being prepared.