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Growth and X –Ray Characterization of $ScFe_4Al_8$ Single Crystals

Single crystals of the $ScFe_4Al_8$ intermetallic compound were obtained by the Czochralski method from a levitated melt. The X–ray powder diffraction, Laue and Berg–Barrett reflection topographies exhibit that the obtained single crystals were a good quality. The lattice parameters a = 8.652 ± 0.004 Å, c = 5.020 ± 0.003 Å were calculated from powder diffraction patterns.

Keywords: intermetallic compound, single crystal growth, X-ray topography

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1. Introduction

There is a large family of the tetragonal RT_xM_{12-x} compounds, where R is rare earth or actinide element, with $ThMn_{12}$ type structure. These materials are formed in principle as ternaries and they can be divided into two distinct subgroups: the first one with high concentration of transition element T and the second one with lower concentration of T ranging from x = 4 to 6. The representatives of the first group are potential interesting magnetic materials, whereas the members of the second group, $ScFe_4Al_8$ among them, exhibit puzzling physical properties. For determination of physical properties one needs single crystalline material.

The $ThMn_{12}$-type tetragonal compounds existing mostly as ternaries or pseudoternaries have caused recently a considerable interest both from the fundamental point of view (heavy fermion-like compounds) and as potential hard magnetic materials (alloys with a high concentration of Fe or Co) (for review, see SUSKI et al.). In the $ThMn_{12}$-type of structure (the space group I4/mmm) there are four inequivalent crystallographic positions: the 2(a) which are occupied by the rare earth (Sc) or actinide atoms, whereas in the 8(f), 8(i) and 8(j) sites other atoms are distributed. In the RFe_4Al_8-type compounds the iron atoms are located in principle in the 8(f) position. These atoms form antiferromagnetic sublattice but the detailed magnetic ordering exhibits various modifications even for nonmagnetic rare earths (SCHOBINGER-PAPAMANTELLOS et al.). Sc like Y can be used as nonmagnetic component in reference compounds to determine the contribution of the f-electron element to the magnetism of intermetallics. $ScFe_4Al_8$ is antiferromagnetic below about 120 K, following a Curie-Weiss law at higher temperatures; however, at low temperature in magnetic field above ~10 T it exhibits apparent saturation (KOTUR et al.). The temperature dependence of the electrical resistivity shows a clear metallic character (KOTUR et al.). Therefore, to elucidate the physical properties of this material a single crystal sample is indispensable. The polycrystalline sample of $ScFe_4Al_8$ has been obtained as described by KOTUR et al.

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2. Crystal growth

The $ScFe_4Al_8$ single crystals were grown by the Czochralski method from a levitated melt using the previously starting elements melted together (ingot ~ 1.5g). The growing chamber was evacuated with a high vacuum unit and filled with pure argon several times. The starting polycrystalline samples were heated to red hot to remove any absorbed gases. The molybdenium spike was immersed in the melt and withdrawn at a velocity of about 10 mm/h. By increasing of temperature, necking down of the growing crystal was obtained to ensure the growth of a single crystal. The obtained single crystals have a cylindrical shape with a length of 10 mm and about 1.5 mm in diameter (Fig. 1.).

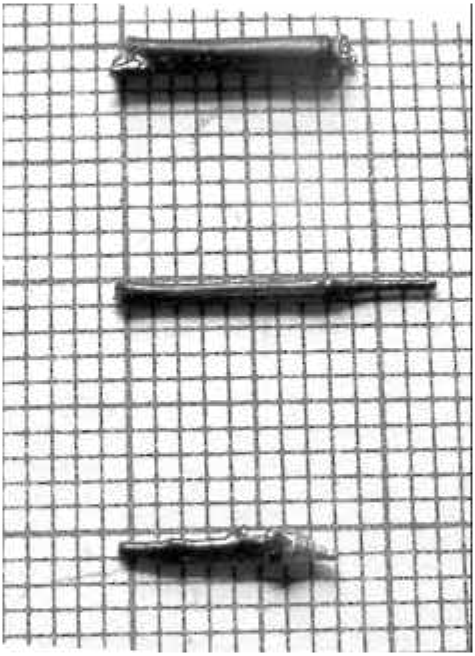

Fig. 1: As grown $ScFe_4Al_8$ single crystals on the millimetre scale.

3. X–ray investigations

A part of a single crystal was powdered in an agate mortar. X-ray diffraction pattern of powdered sample was recorded using a Powder Diffractometer D5000 from Siemens. The obtained X-ray spectrum confirmed existence of the $ThMn_{12}$ crystal structure of the investigated crystal (Fig. 2.).

The calculated lattice parameters are $a = 8.652 \pm 0.004$ Å, $c = 5.020 \pm 0.003$ Å. The Laue method showed the obtained crystals were single crystals and the Laue spots pointed to good quality of the crystals. The orientation of the crystals was also found. The growth direction for one of the single crystals was found to be [100]. The Laue pattern with the 2mm symmetry in displayed in Fig.3.

As grown crystals were examined by X-ray reflection topography (Berg-Barrett topography) with the use of Fe K_α radiation. The diffraction angle 2θ was chosen to be close to 90^o. The distance between the crystal and the photographic plate was about 1 mm. High resolution D2 photographic plates from AgfaGevaert were applied. Berg–Barrett topograph of the $ScFe_4Al_8$ single crystal is shown in Fig.4.

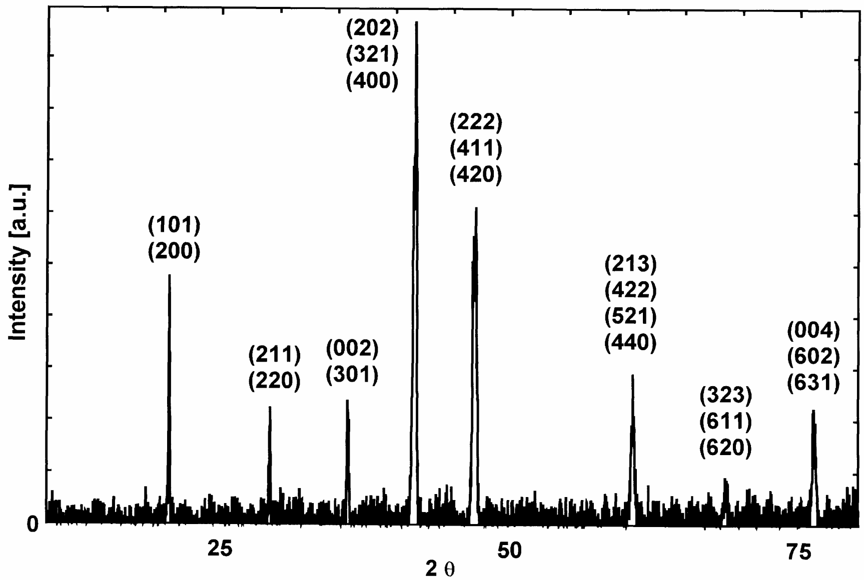

Fig. 2: The powder diffraction pattern of $ScFe_4Al_8$.

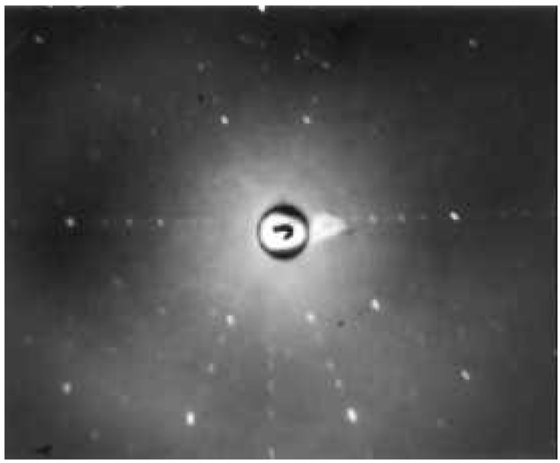

Fig. 3: X-ray Laue pattern (backscattering), 2mm symmetry.

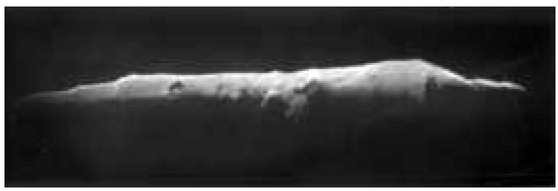

Fig. 4: The Berg-Barrett topography of $ScFe_4Al_8$ single crystal.

Some of the examined crystals exhibit mosaic structure. The mosaic blocks with the dimension of a few millimetres were elongated along the growth directions. These mosaic samples consist of blocks which may have a slightly different atomic concentration. Their diffraction lines of the powder pattern were broadened in comparison with the powdered the good quality single crystal.

4. Some general remarks

The shape of the crystals grown by the Czochralski method was very convenient for measurements, e.g. electrical resistivity, magnetic susceptibility (dc and ac), magneto-crystalline anisotropy etc. The Czochralski method from a levitated melt allows obtaining good quality of the $ScFe_4Al_8$ single crystals using small amounts of ingot. The best quality fragment of crystals, as determined by the Berg–Barrett topography, will be used for further investigations of the physical properties.

Acknowledgements

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