

11.7 Electron Density and Potential Distribution in GaN from X-Ray Diffraction Experiment

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The method of the evaluation of the electrostatic potential in a crystal by X-ray diffraction is discussed. The distribution of the electrostatic potential in GaN is discussed with the reference to the charge distribution.

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11.8 Modulated Magnetic Structure of ScFe₄Al₈ by X-Ray, Neutron Powder Diffraction and Mössbauer Effect

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The ternary intermetallic ScFe₄Al₈ alloy presented in this paper belongs to the extensively investigated ThMn₁₂-type family, reviewed recently in Refs. [1, 2]. The diffraction investigations confirm the *bc* structure I 4/mmm (*a*~860 pm, *c*~499 pm at RT) in which four non-equivalent crystallographic sublattices are present. As was shown, the iron sublattice - (8f) in this family of alloys can exhibit very complicated magnetic properties [1]. Depending on the main metal at (2a) positions, uranium, thorium or scandium, the magnetic moments in Fe sublattice (8f) form double modulated spiral structure [1], spin-canted system [2] or a single-*q* spiral which we find for ScFe₄Al₈. In the latter alloy, in contrast to the one containing uranium or thorium, we could expect relatively low magneto-crystalline anisotropy. The unpolarized neutron diffraction pattern leaves no doubts that the modulated magnetic structure is observed in the tetragonal ScFe₄Al₈ compound. The interpretation of our neutron data requires the presence of non-zero magnetic propagation vector different from the nuclear one. The iron magnetic moments of ScFe₄Al₈ sample create a

spiral structure with spins rotated in a plane parallel to the wave vector $q = (q_x, q_x, 0)$, with $q_x = 0.136(2)$ which is temperature independent up to 187 K. The value of the iron magnetic moment at 8 K is close to 1.08(12) μ_B . The basic magnetic cell has to be purely antiferromagnetic with iron spins directed along *a* or *b* axis and rotated in the basal plane by $49(1)^\circ$ from cell to cell. The antiferromagnetic nature of ScFe₄Al₈ is fully confirmed by Mössbauer measurements. The neutron data also show that scandium doesn't contribute to the magnetism of ScFe₄Al₈.

- [1] K. Rečko et al., Phys. Stat. Sol. (2002) in press
 [2] K. Rečko et al., J. Alloys Comp. 334, 1-2(2002)58

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11.9 Magnetic Properties of Sc(FeAl)₁₂ Samples by Powder Diffraction Techniques and Mössbauer Effect

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X-ray and Neutron Diffraction techniques allowed us to determine crystallochemical structure of ScFe₄Al₈, ScFe₅Al₇ and ScFe₆Al₆ alloys with I4/mmm symmetry, isostructural to ThMn₁₂-type structure. Magnetic properties of ScFe₄Al₈ and ScFe₆Al₆ powder samples are presented. These alloys have been measured by means of conventional Mössbauer Effect (ME) as well as by Monochromatic Circularly Polarized Mössbauer Source (MCPMS). The results of Mössbauer experiments are compared with the neutrons data conclusions regarding the magnetic structure. ScFe₄Al₈ alloy orders around 250 K by forming antiferromagnetic spiral iron

sublattice within the tetragonal basis plane *ab* and magnetic iron moment close to 1.1(2) μ_B at 8 K.

- [1] K. Rečko et al., Phys. Stat. Sol. (2002) in press
 [2] K. Rečko et al., J. Alloys Comp. 334, 1-2(2002)58

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