THE REFINEMENT OF β-Fe_6Ga_5 CRYSTAL STRUCTURE*

T.N. VERSHININA[1], I.A. BOBRIKOV[1], S.V. SUMNIKOV[1], A.O. BOEV[2], A.M. BALAGUROV[1],

A.K. MOHAMED[3], I.S. GOLOVIN[3]

[1] *Joint Institute for Nuclear Research, Dubna, Russian Federation*
[2]*Belgorod National Research University, Belgorod, Russian Federation*
[3]*NationalUniversity of Science and Technology "MISIS", Moscow, Russian Federation*

Magnetostrictive materials, such as Fe-Ga alloys, are a type of functional materials, the main feature of which is the interaction of magnetic and mechanical energy when an external magnetic field or stress is applied. Ferromagnetic alloys based on the Fe-Ga binary system have highest saturation magnetostriction among iron-based alloys [1]. These alloys are used for the manufacture of pressure sensors and sonars due to a good combination of functional and mechanical properties.

Low-temperature diffusion-controlled phase transformations in alloys of the Fe-Ga system proceed slowly. This helps to maintain at room temperature nonequilibrium high-temperature phases, which were formed during crystallization from the melt. The structure of the Fe-45at.%Ga alloy quenched from the melt is β-Fe_6Ga_5. This phase exists in a narrow temperature range of 770–800°C according to the equilibrium diagram of Fe-Ga [2]. The crystal structure of the β-Fe_6Ga_5 has been refined using the R-3m space group in [3] were it was called as ζ_2-GaFe.

In our studies, neutron and X-Ray diffraction patterns were measured for several samples of the Fe-45Ga alloy in different states. Dependently on heat treatment the structure changed from single to multiphase state. In the paperthe refinements of crystal structure for all studied samples will be presented as well as density functional theory calculations. In Fig. 1 a preliminary result of the Rietveld refinement is shown, where good agreement between experimental and calculated values is seen.

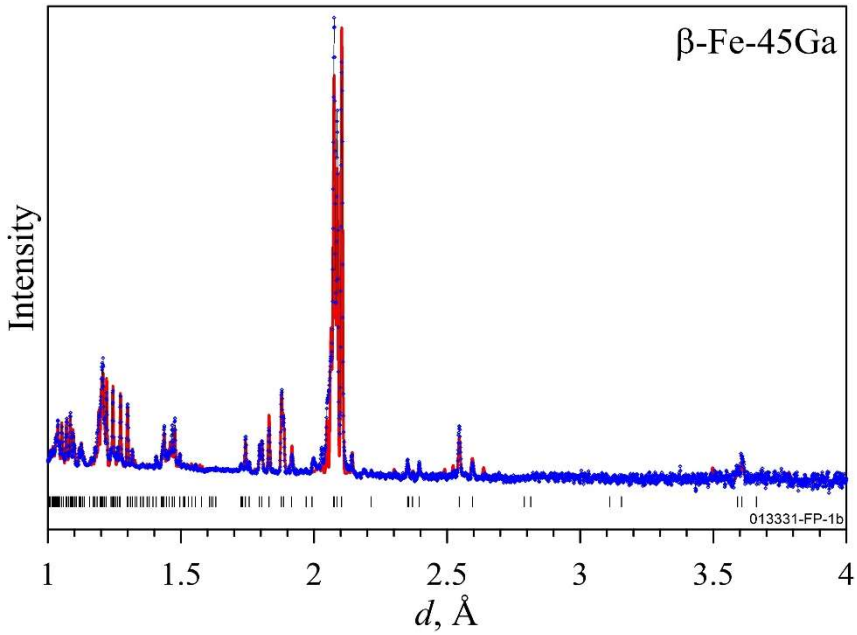

Fig.1. Neutron diffraction pattern for as cast Fe-45Ga alloy measured at room temperature and processed by the Rietveld method. Experimental points and calculated line are shown. The vertical bars indicate calculated peak positions of the β-Fe_6Ga_5.

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