Simulation of Structural Defects and Strains in a Single Crystal $Nd_3Ga_5O_{12}$

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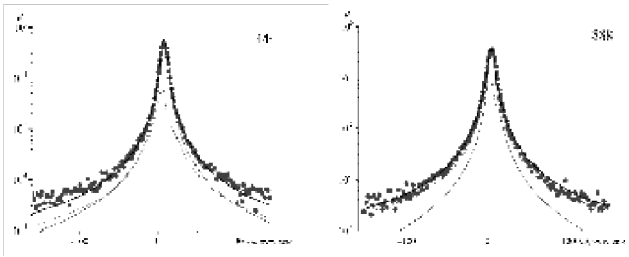
Experimental diffraction reflection curves (DRC) single crystal neodymium-gallium garnet (NGG) differ significantly from the theoretical diffraction for a perfect crystal despite correct account of thermal Debye-Waller factor. In this regard, assumed the presence of a crystal dislocation loops in addition, another type microdefects - spherical clusters (particle inclusions of another phase). Considering the presence of crystal clusters and dislocation loops at the same time was much more successful (Fig. 1), however, the simultaneous adjustment of both DRC at default dislocation loops (R=100 nm, N= $8\cdot10^{11}$ cm^{-3}) and only one cluster radius was satisfactory only in certain areas of the measured angular ranges.

But setting two radii of clusters identical for the two reflexes (R=10 i 50 nm) by changing the concentration of clusters (respectively N= $5\cdot10^{13}$ i $5\cdot10^{11}$ cm^{-3}) and a fixed value of the parameter deformation on the edge of the cluster (ε =0.03) allowed better performance fit with existing statistical dispersion measurements, when the corresponding figures up μ=12%, R_w=18% i μ=14%, R_w=17% for the 444 and 888 reflections.

Fig.1.Experimental and theoretical diffraction NGG (markers and thick solid lines) for reflections (444) and (888). The thin solid and dashed lines - coherent components DRC and contributions from diffuse scattering clusters and dislocation loops



Thus, obtained in our work a good quality fit for each of the measured DRC diffraction in the central parts and in the tails achieved of adequate and self-consistent description coherent intensity and diffuse scattering using generalized statistical dynamical theory of X-ray diffraction in single crystals with uniformly distributed micro-defects [1].

1. X-ray diffractometry dynamic defect structure garnet single crystals/ [V.M. Pylypiv, B.K. Ostafiychyk, T.P.Vladimirova, Ye.M. Kyslovskyy, V.B. Molodkin, S.I. Olikhovskii, O.V. Reshetnyk, O.S. Skakunova, V.V. Lizunov] // Nanosystems, nanomaterials and nanotechnologies. – 2011. – V. 9, № 2. – P. 375-408.