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I.A. Kaurova, E.N. Domoroshchina, G.M. Kuz'micheva, V.B. Rybakov

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Evaluation of stability region for scandium-containing rare-earth garnet single crystals and their congruent-melting compositions

I.A. Kaurova[1], E.N. Domoroshchina[1], G.M. Kuz'micheva[1], V.B. Rybakov[2]

[1] *Department of Materials Science and Technology of Functional Materials and Structures, Moscow Technological University, MITHT, Vernadskogo pr. 86, Moscow, Russia*

[2] *Department of Chemistry, Lomonosov State University, Vorobyovy Gory 1, Moscow, Russia*

e-mail:kaurchik@yandex.ru

Abstract

Single crystals of scandium-containing rare-earth garnets in system *R*-Sc-*C*-O (R^{3+} = Y, Gd; C^{3+} = Al, Ga) have been grown by the Czochralski technique. X-ray diffraction analysis has been used to refine crystal compositions. The fundamental difference between the melt compositions and compositions of grown crystals has been found (except for compositions of congruent-melting compounds, CMC). The specific features of garnet solid solution formation have been established and the ternary diagrams with real or hypothetical phases have been built. The dinamics of coordination polyhedra changes with the formation of substitutional solid solutions have been proposed based on the mathematical modeling and experimental data. Possible existence of CMC with garnet structure in different systems as well as limit content of Sc ions in dodecahedral and octahedral sites prior to their partial substitution of ions, located in other sites, have been evaluated. It was established that the redistribution of cations over crystallographic sites (antistructural point defects) due to system self-organization to maintain its stability may be accompanied by cation ordering and the symmetry change of individual polyhedrons and/or the whole crystal.

Keywords: A1. Solid solutions; A1. X-ray diffraction; A1. Phase diagrams; A2. Czochralski method

1. Introduction

Compounds and solid solutions of single-crystal garnets are widely used in optoelectronics as active elements of lasers, magneto-optical media for controlling light irradiation, solid-state luminescent dosimeters, fluorescent detectors, and LED phosphors [1,2].