Influence of Al, Ga and In on the Crystal Structure of $ErGe_{2\pm x}$

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Samples of digermanides of rare-earth elements are frequently prepared by the flux method using indium, gallium or aluminum flux. We decided to undertake a systematic investigation of the influence of small quantities of Al, Ga and In on the crystal structure of "digermanides" in an extended sense ($RGe_{2\pm x}$).

The existence of the compounds $ErGe_{2.83}$, Er_2Ge_5, $ErGe_{1.83}$, $ErGe_{1.5}$, and Er_3Ge_4 was confirmed in the range 20-40 at.% Er of the binary system at 600°C.

The addition of small quantities of Al leads to the formation of substitutional solid solutions for Er_2Ge_5, $ErGe_{1.83}$ and Er_3Ge_4 (up to 2, 3 and 5 at.% Al, respectively). On the contrary, the solid solution based on $ErGe_{1.5}$ displays a progressive filling-up of the vacancies in the AlB_2-type binary structure (up to 5 at.% Al). $ErGe_{2.83}$ does not dissolve any significant amount of Al. The crystal structure of the ternary compound $ErGe_{1.85}Al_{0.15}$ ($ZrSi_2$-type structure, Pearson symbol *oS*12, *Cmcm*, a = 4.0490(2), b = 15.9791(7), c = 3.9102(2) Å) was determined by X-ray powder diffraction.

The addition of Ga causes the formation of larger solid solutions, which can be explained by the similar values of the atomic radii of Ga and Ge. The existence of $ErGe_{1.85}Ga_{0.15}$ with a $ZrSi_2$-type structure was confirmed. The formation of a ternary compound of composition $Er(Ga,Ge)_3$ was established. Its crystal structure can be derived from the defective $ErGe_{2.83}$ structure. No significant solubility of indium in binary erbium germanides was observed.

Keywords: rare-earth germanide, solid solution, crystal structure