SYNTHESIS AND X-RAY DIFFRACTION RESEARCH OF
\( \text{V}_{0.25}\text{Fe}_{0.75}\text{InS}_3 \) AND \( \text{V}_{0.75}\text{Fe}_{0.25}\text{InS}_3 \)

I.B. ASADOVA, G.G. GUSEYNOV, O.M. ALIYEV

Inorganic and Physico-Chemistry Institute of Academy of Sciences, Azerbaijan, Baku

Introduction

Synthesis of highly anisotropic semiconductor compounds with magnetic ions, learning of their physicochemical and structural specifications on the single crystal samples, detection of phasing and principles of structural transitions in them has great scientific and practical significance.

From this point of view this work is dedicated to synthesis, growths of single crystals and structural researches of phases, forming in the system (Ga In\(_S\_3\)Fe). For detection of phasing in the system and margins of stability of the structure of phases were synthesized \( \text{Ga}_{0.25}\text{Fe}_{0.75}\text{InS}_3 \) and \( \text{Ga}_{0.75}\text{Fe}_{0.25}\text{InS}_3 \).

Method

Synthesis was conducted by the direct method from elements in the evacuated quartz ampoules at the temperature 1050°C. Rising of temperature to 650°C with the speed 100°/hour, 3-hours ageing at this regime and slow rising of temperature to 1050°C. After 40 minutes of ageing the ampoules have been cooled slowly to 550°C and homogenized at this regime during a week.

Conclusion

As synthesized samples are not laminated, it is considered, that they are ordered phases on the base of structure (GaInS\(_3\)).

It is known that the ordering of the structures takes place with the multiplying of one of the parameters of screen on 2,3,4... \( \times 2, \times 3 \) and so on, it was decided to calculate \( d \) for whole setting of diffraction reflections with the purpose of finding of indexes hkl on the base of one of indicated variations. However these attempts were not successful. Therefore it was determined by the analytical way that symmetry of crystals is not trigonal and reflections not stowed into these system require more low symmetry. Thus, it is determined that these phases are isostructural and crystallize in rhombic syngony with the group of symmetry Pnnm.

\( \text{Ga}_{0.25}\text{Fe}_{0.75}\text{InS}_3 \) \( a=3.82; b=4.475; c=12.189 \) \( \text{Ga}_{0.75}\text{Fe}_{0.25}\text{InS}_3 \) \( a=3.90; b=4.479; c=12.272 \).

Taking into consider the facts that for sulphides of every stechometry and structural type the volume for one atom of sulfur makes average \( \approx 40A \) (\( V_s=V/\sum S \) in screen) it was calculated the contents of screen of investigated crystals. It was found that the structure is defective in result of statistic distribution of most part of atoms of metals, number of units in the screen makes 1,666. On the base of this the structural formula corresponds with 1,666 (Ga\(_1\), Fe\(_x\)InS\(_3\)). In this case quantity of sulfur in the screen makes 5 and \( V_p=41A \) from at the rate of \( V_p=212A^3 \).

Thus, it is determined that at the partial replacement of tetraedryl atoms Ga in structure GaInS\(_3\) with the atoms of Fe in wide interval of concentration \((0.15+0.75)\) isostructural series of Ga\(_{1-x}\)Fe\(_x\)InS\(_3\) type formed.