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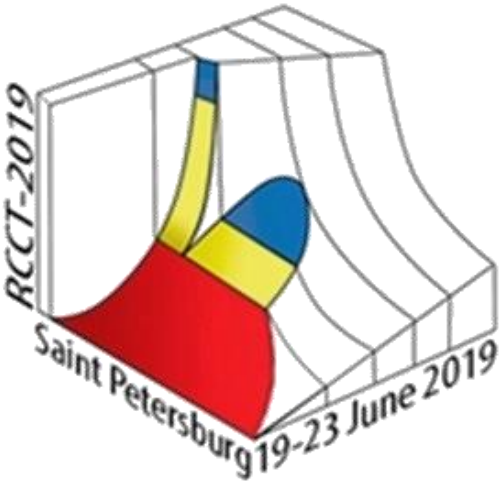

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BOOK OF ABSTRACTS

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PI-53. Thermodynamic Modeling of the Behavior of A^2B^6 Compounds in a Wide Range of Temperatures and Pressures

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Semiconductor compounds of the A^2B^6 group are promising materials to creation of unique instruments of optics, optoelectronics, acoustoelectronics, nanoelectronics, laser technology, detecting ionizing radiations. For example, zinc selenide crystals are increasingly applied in the infrared, LED, and fiber optic technology as the detectors of X-rays and elementary particles. Crystals of zinc chalcogenides (ZnSe and ZnS) doped with ions of transition metals (Fe^{2+}, Co^{2+}, Cr^{2+}) are promising materials for creating active media of tunable solid-state lasers.

For growing crystals it is necessary to know the properties of these materials in liquid and solid states. It should be noted that physical and chemical properties of A^2B^6 compounds and alloys are investigated good enough in solid state. However, for liquid phase the information is lack. This is due to the great difficulties in working with these substances: high melting points, high pressures of own vapors, chemical aggressiveness of the gas phase and melts, toxicity. The lack of data constrains the development of all technologies for obtaining these materials, which, in turn, limits the possibilities of their practical application.

In the present work using the TERRA software [1] and thermodynamic modeling method [2] the thermodynamic characteristics and equilibrium composition of the condensed and gas phases formed during the equilibrium heating of ZnSe, ZnS, CdSe, CdS, in wide range of temperatures (300-3000 K) at different common pressures (1, 10, 10^2, 10^3, 10^4, 10^5, 10^6, 10^7, 10^8, 10^9 Pa) in an argon atmosphere were studied. Temperature dependences of the content of condensed and gas phases and thermodynamic state parameters for each of the systems studied over a wide temperature and pressure ranges have been constructed.

[1] B.G. Trusov, *Vestnik of Bauman Moscow State Technological University*, 2012, Vol. 2 (special Issue), 240.
[2] N.A. Vatolin, G.K. Moiseev, B.G. Trusov, *Thermodynamic modeling in high temperature inorganic systems*, 1994, Metallurgia, Moscow (in Russian).