Computer Modeling of Local Structure and Properties of Oxide Solid Solutions with NaCl Type Structure

Tatiana G. Petrova, Vadim S. Uruosv, Nikolai N.Eremin, *Department of Geology, Moscow State University, Russia.* E-mail: t_petr@mail.ru

Atomistic semi-empirical potentials were applied to calculate the structural, thermodynamic, elastic properties and phase equilibrium of MgO-CaO, MgO-MnO, MnO-CaO, CaO-SrO, BaO-SrO disodered solid solutions by using of the GULP code [1]. The calculations were performed with partially covalent approximations for 7:1, 3:1, 1:1, 1:3, 1:7 randomly mixed cation compositions. It was used 256-ion primitive supercell with quadrupled parameters of the unit cell for all compositions. It was demonstrated that such supercell allows to imitate random distribution of cations.

On the basis of the calculated values of free energy the component fields of stability, mixing limits and critical temperature were predicted. The values are in a good agreement within the temperature range 298 – 1800 K with the available data and results of other theoretical investigation. For 1:1 composition the analyses of the local structure (interatomic distances and atomic displacements) from regular positions structure was perfomed. In particular, the insignificant shifts of cations and the essential shifts of anions from the initial ideal positions of the supercell were established [2], [3].

[1] Gale J., *GULP user manual*, Royal institution and Imperial College, London, 1992. [2] Urusov V.S., Petrova T.G., Eremin N.N., *D. Akad. Nauk*, 2002, **47**, 811. [3] Urusov V.S., Petrova T.G., Eremin N.N., *D. Akad. Nauk*, 2003**, 392**, 469.

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