

Synthesis of rock-salt ZnO-LiMeO₂ solid solutions (Me = Sc³⁺, Ti³⁺, Fe³⁺, In³⁺) at high pressure and high temperature

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Zinc oxide belongs to the family of wide-band-gap semiconductors and possesses high exciton binding energy (60 meV). At ambient conditions ZnO has a hexagonal wurtzite structure (space group P6₃mc) which transforms into cubic rock-salt one (space group Fm3m) at pressures above 6 GPa and reverts to wurtzite phase at pressure release. Recently a number of metastable Me_{1-x}Zn_xO solid solutions (Me^{II} - Ni²⁺, Fe²⁺, Co²⁺, Mn²⁺) with rock-salt structure have been synthesized by quenching from 7.7 GPa and 1450-1650 K [1]. Quenched Ni_{1-x}Zn_xO rock-salt solid solutions show remarkable stability at ambient conditions in a wide concentration range (0 < x ≤ 0.8) [1].

In the present work we report the synthesis of metastable rock-salt (LiMeO₂)_{1-x}(ZnO)_x solid solutions (Me = Sc³⁺, Ti³⁺, Fe³⁺, In³⁺) obtained in the wide concentration range up to x=0.8 by quenching from 7.7 GPa and 1350-1550 K. Lattice parameters of solid solutions have been calculated from X-ray diffraction patterns taken at temperatures up to 1073 K on B2 beamline (HASYLAB-DESY). It was found that the lattice parameters of all synthesized rock-salt solid solutions perfectly follow the Vegard's law. Samples with x>0.8 consist of two-phase mixtures of solid solutions with wurtzite and rock-salt structure. As was shown in the series of preliminary experiments at ambient pressure concentration range of rock-salt (LiFeO₂)_{1-x}(ZnO)_x solid solutions is limited for x<0.3, thus the synthesis at high pressure and high temperature substantially extends the concentration range of rock-salt phase.

For all the studied systems the onset of thermal decomposition depends on concentration. For example, at x=0.8 (LiFeO₂)_{1-x}(ZnO)_x rock-salt phase is stable at ambient pressure up to 673 K, but at x=0.6 temperature increases up to 773 K. The nature of Me³⁺ cation seriously influence on the thermal stability of rock-salt phase too. Rock-salt solid solution (LiScO₂)_{0.3}(ZnO)_{0.7} is stable up to 823 K whereas of (LiFeO₂)_{0.3}(ZnO)_{0.7} is stable up to 723 K.

[1] A.N. Baranov, P.S. Sokolov, O.O. Kurakevych, V.A. Tafeenko, D. Trots, V.L. Solozhenko, High Press. Res. 2008, **28**, 515.

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