Atomic and electronic structures of interfaces in oxide glass-ceramic composites

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Oxide glass ceramics are composite materials in which oxide micro/nano crystallites are incorporated into matrix of oxide glass. The interest in studying of such kind of materials is related to wide prospects of their potential applications, in particular, in electronics, optical thermometry, biomedicine, etc [1]. The physical properties of glass-ceramic materials are largely determined by electronic properties of the "interphase region", which has an atomic structure different from the structure of both crystalline and glass components. The physical characteristics of interphase regions of composite materials are difficult to predict using only general ideas about atoms, ions or molecules interactions. However, the mutual diffusion of component atoms can be effectively modeled in calculations using the molecular dynamics (MD) methods. Further application of the electronic structure calculation methods to the obtained atomic structures allows to calculate the most important micro- and macro-characteristics of the interphase layers and thus to explain the experimentally observed properties of glass-ceramic composites.

This work presents results of complex computational and experimental studies of the atomic and electronic structures of interphases of oxide glass-ceramic composite materials of two different types: a) $K_2Bi(PO_4)(WO_4)$ crystal in K_2O-P_2O_5-WO_3-V_2O_5 phosphate-tungstate glass system; b) $LaVO_4$ crystal in (1-x)B_2O_3-xV_2O_5 and xLi_2O-2V_2O_5-(98-x)B_2O_3 borate glass systems. The atomic structures of interface layers of composites were calculated by MD methods implemented in Amorphous Cell and Forcite programs of Materials Studio software package [2]. The electronic structure calculations were performed in the DFT approximation using the band-periodic plane wave pseudopotential method CASTEP.

Obtained computational results are compared with experimental data on structural analysis, optical and luminescence spectroscopy of pure and RE-doped samples of glass-ceramic composite materials. A relationship between atomic and electronic structures of interface (interphases) layers and optical characteristics of studied composites is analyzed. The possibility of tuning of the optical properties of studied oxide glass-ceramic composite materials is discussed.

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