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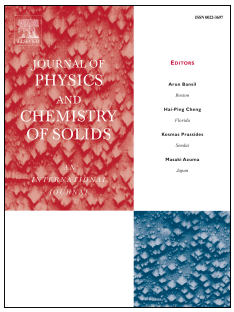

Theoretical study of the local structures and the EPR parameters for RLNKB glasses with VO^{2+} and Cu^{2+} dopants

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Theoretical study of the local structures and the EPR parameters for RLNKB glasses with VO^{2+} and Cu^{2+} dopants

Chang-Chun Ding [*] [a], Shao-Yi Wu [*] [a], Li-Na Wu [a], Li-Juan Zhang [a], Li Peng [a], Ming-He Wu [a], Bao-Hua Teng [a]

[a] Department of Applied Physics, School of Physical Electronics, University of Electronic Science and Technology of China, Chengdu 610054, PR China

Abstract: The electron paramagnetic resonance (EPR) parameters and local structures for impurities VO^{2+} and Cu^{2+} in RO-Li_2O-Na_2O-K_2O-B_2O_3 (RLNKB; R = Zn, Mg, Sr and Ba) glasses are theoretically investigated by using the perturbation formulas of the EPR parameters for tetragonally compressed octahedral $3d^1$ and tetragonally elongated octahedral $3d^9$ clusters, respectively. The VO^{2+} and Cu^{2+} dopants are found to undergo the tetragonal compression (characterized by the negative relative distortion ratios $\rho \approx -3\%$, -0.98%, -1% and -0.8% for R = Zn, Mg, Sr and Ba) and elongation (characterized by the positive relative distortion ratios $\rho \approx 29\%$, 17%, 16% and 28%), respectively, due to the Jahn-Teller effect. Both dopants show similar overall decreasing trends of cubic field parameter D_q and covalency factor N with decreasing electronegativity of alkali earth cation R. The conventional optical basicities Λ_{th} and local optical basicities Λ_{loc} are calculated for both systems, and the local Λ_{loc} are higher for Cu^{2+} than for VO^{2+} in the same RLNKB glass, despite the opposite relationship for the conventional Λ_{th}. This point is supported by the weaker covalency or stronger ionicity for Cu^{2+} than VO^{2+} in the same RLNKB system, characterized by the larger N in the former. The above comparative analysis on the spectral and local structural properties would be helpful to understand structures and spectroscopic properties for the similar oxide glasses with transition-metal dopants of complementary electronic configurations.

Keywords: RO-Li_2O-Na_2O-K_2O-B_2O_3; Electron paramagnetic resonance (EPR); Defect structures: VO^{2+} and Cu^{2+}