

EFFECT OF RADIATION DEFECTS ON THE ELECTRONIC STRUCTURE OF ZIRCON BY X-RAY PHOTOELECTRON SPECTROSCOPY DATA

Yu. V. Shchapova,¹ S. L. Votyakov,¹ M. V. Kuznetsov,²
and A. L. Ivanovskii²

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X-Ray photoelectron spectroscopy (XPS) is used to study the electronic structure of radiation damaged samples of ZrSiO_4 zircon mineral at early and middle stages of its radiation destruction. The effects of radiation induced atomic disordering are found to be most distinctly manifested in the spectra of $\text{O}1s$ states and to a smaller extent in the spectra of $\text{Si}2p$ states, and also in the zircon valence band. Based on the quantum chemical calculation results the conclusion is drawn that the observed changes in XPS lines are caused by the formation of oxygen vacancy defects and an increase in the covalency of interatomic bonds near oxygen vacancies. For zircon samples with a low/moderate degree of radiation damage these changes reflect the initial stage of the polymerization of the ZrSiO_4 structure due to the formation of Si-O-Si chain fragments.

Keywords: zircon mineral, radiation defects, electronic structure, XPS.