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XANES study of Chromium-Rare-earth Zircons and Sheelites

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Abstract content

The mixed oxide RCrO4 (R3+= Er and Y) crystallizes into a tetragonal zircon-type structure at ambient conditions. It is built from edges-sharing RO8 dodecahedra chains which are connected each other by CrO4 tetrahedra. Under high pressure conditions (50 kbar), scheelite polymorphs (S.G. I41/a) [1, 2] of RCrO4 were prepared from the corresponding zircon forms of RCrO4 (S.G. I41/amd). Chromium in these materials shows relative rare Cr5+ oxidation state. Bulk magnetic and specific heat measurements indicate the presence of antiferromagnetism with estimated Néel temperatures of 23 and 21 K respectively. However, the RCrO4-zircon type polymorphs show ferromagnetic behavior with Curie temperatures of 15 and 9 K. The differences in the magnetic behavior of both forms have been attributed to the changes found in the Cr-O-R superexchange pathway through which the magnetic interactions take place. To contribute clarifying the mentioned behavior, XAFS measurements on Cr K-absorption edge were performed at Stanford Synchrotron Radiation Lightsource, at beamlines 2-3 and 4-3. The pre-edge feature in the XANES zone is markedly detected. The shift in the energy position between the pre-edge peak and the “shoulder” of the XANES region is about 5.5-6 eV, in agreement with reported data for Cr(V) oxidation state [3]. From the crystal structure reported by XRD, an ab initio modeling with FEFF8.4 code of XANES spectra has been performed and the density of states of ions was also obtained. The modeled spectra qualitatively reproduce the main features of the experimental ones.

Summary

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