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High-temperature Mössbauer study of Fe-substituted mullite

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ABSTRACT

Mössbauer spectra of Fe-substituted 3/2-mullite (10.3 wt% Fe_2O_3) have been measured from room temperature up to 1200 °C under nitrogen atmosphere. A Voigt-type fit to the spectral line shape is proposed that is based on the assumption of three non-equivalent Fe^{3+} environments A, B, and C in the mullite structure. The Fe^{3+} subspectra display quadrupole splittings of about 1.1 (A), 0.7 (B), and 1.3 mm/s (C) where the isomer shifts at room temperature are about 0.3 mm/s for subspectrum A and B and about 0.1 mm/s for site C. Subspectrum A and B are attributed to two different Fe^{3+} octahedral sites in mullite coordination, experiencing slightly different quadrupolar interactions; the third site is assigned to ions in tetrahedral coordination. Subspectrum A is assigned to the iron-oxygen octahedra having TO_4 tetrahedra as next nearest neighbors, while subspectrum B may correspond to iron-oxygen octahedra having TO_4 and T^*O_4 tetrahedra with associated oxygen vacancies in their vicinity. The quadrupolar splittings of the three subspectra are found to be almost independent of temperature. The temperature dependences of the isomer shifts conform closely to those expected for a harmonic solid at the high-temperature limit. The Mössbauer study gives no support for any temperature-induced redistribution of Fe in mullite.