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INFRARED BAND ASSIGNMENT OF AL-SI MULLITE AND SiO_2-FREE COMPOUNDS WITH MULLITE STRUCTURE

by

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Mullite is an aluminium silicate with the general formula $Al_2[Al_{2+2x}Si_{2-2x}]O_{10-x}$, where x denotes the number of oxygen vacancies per unit cell. SiO_2-free phases with mullite structure can be obtained by the substitution of silicon by germanium and aluminium by gallium, or by addition of alkali metal ions for charge compensation of a mullite-type Al_2O_3. FTIR spectroscopic investigations were performed on synthesized powders of Al-Si, Al-Ge, Ga-Ge and alkali (Na, K, Rb) aluminate mullites. The IR spectra of Al-Si mullite and the germanate mullites in the lattice vibration region (1400 - 400 cm^{-1}) are characterized by the presence of three main band groups, which are located for Al-Si mullite in the (a) 1200 - 1100 cm^{-1}, (b) 1000 - 700 cm^{-1} and (c) 650 - 400 cm^{-1} spectral range. For Al-Ge and Ga-Ge mullites these band groups show a strong shift towards lower wavenumbers, which can be explained with the increasing size of the polyhedra in the substituted mullites. In IR spectra of the alkali aluminates only two band groups, (b) and (c), are observed, which are also shifted to the low energy region compared to Al-Si mullite due to increased Al–O distances [1]. The IR spectrum of the Na aluminate mullite exhibits a fine structure, which continuously vanishes in a solid solution from Na- to K-Al mullite. It can be assumed, that ordering effects are responsible for the more complex band structure of the Na aluminate.

The infrared absorption bands of the mullite-type compounds were deconvoluted into a minimum number of nine single bands. On the basis of observed band shifts and the polarization behaviour of a mullite single crystal [2, 3] the following assignment for the infrared bands of mullite is proposed: Bands in the high energy region (a) are assigned to Si–O and Ge–O stretching vibrations, mainly occuring along the short (Si, Ge)–O bond within the (001) plane. The absence of group (a) bands in the mullite-type silica-free alkali aluminates strongly supports this interpretation. Group (b) bands are mainly determined by stretching vibrations of Al and Ga on tetrahedral sites and T–O–T bending vibrations. The bands of group (c) can be assigned to stretching vibrations of Al and Ga in octahedral coordination and to O–T–O bending vibrations.

References

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