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HYDROXYL IONS IN SYNTHETIC CRYSTALS: DO THEY DIFFER FROM THOSE IN MINERALS?

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Synthetic crystals are produced for practical applications where the presence of hydroxyl ions in the material may be either desirable or undesirable. In any case a small amount of OH^- ions in *as-grown* anhydrous crystals (alkali halides, fluoroperovskites, oxides etc.) can easily be detected by the high resolution FTIR absorption technique, if the crystals are grown at high temperatures (600 – 1600 °C) from melt or solution in air atmosphere. Unlike to many cases of minerals, the relatively large single crystal samples do not require special microsampling methods or FTIR microscopes. The information obtained from the vibrational frequency of the OH^- ions, and from the pleochroism of the absorption bands are in general very similar and can be used to determine the structural site of the hydroxyl defect in the crystal lattice.

Two review papers have recently been published on OH^- defects in minerals and synthetic oxide crystals by BERAN & LIBOWITZKY (2003) and WÖHLECKE & KOVÁCS (2001), respectively, which present the main similarities and differences between the two classes of materials. In the present work, the anharmonicity of the stretching mode characteristic for all O-H vibrations, the weak coupling to phonon bands in some complex oxides derived from the temperature dependence of the OH^- bands, and the effect of a structural phase transitions on the O-H vibrational frequency in $LaGaO_3$ crystals will be surveyed. The role of hydroxyl ions in the thermal fixing of holographic gratings in photorefractive materials is also shown, and how the composition of some niobates and tantalates can be characterized by the shape of the OH^- bands.

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References

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