HIGH RESOLUTION INFRARED ABSORPTION SPECTRA OF HYDROXYL RELATED DEFECTS IN $CdWO_4$ SINGLE CRYSTALS

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Cadmium tungstate ($CdWO_4$) is one of the best inorganic scintillator materials. Though crystals are usually grown from high purity melts, they may contain some impurities, e.g. hydroxyl ions (OH^-). To identify the trapping sites for the OH^- ions the infrared absorption spectra related to the O-H stretch modes were studied between 10-300 K by Chirila et al [1]. In undoped crystals they detected several narrow bands at low temperatures (with halfwidths smaller than 0.5 cm^{-1}) in the 3495-3516 cm^{-1} wavenumber range, which could not be perfectly resolved by their spectrometer. The bands were assigned to $Cu^+ - OH^-$, $V_{Cd} - OH^-$, and $h^+ - V_{Cd} - OH^-$ centres exploiting the correlation with EPR data.

In the present work the narrow absorption bands related to the presence of hydroxyl ions in undoped $CdWO_4$ crystals have been remeasured using high resolution spectrometers ($\Delta\nu \leq 0.1$ cm^{-1}). The O-H bond directions for the different hydroxyl centres have been determined from the spectra collected for polarized light propagating along the crystallographic axes of the monoclinic crystal. In addition, the exchange of OH^- for OD^- in heavy water vapour atmosphere has been used to calculate the anharmonicity of the stretch modes.

In our experiments 3 main lines were found at about 3497.07 cm^{-1} (FWHM ≈ 0.18 cm^{-1}), 3512.23 cm^{-1} (FWHM ≈ 0.35 cm^{-1}) and 3517.8 cm^{-1} (FWHM ≈ 0.52 cm^{-1}) in the undoped samples measured at 8 K accompanied by several very weak lines at about 3492.4 cm^{-1}, 3495.7 cm^{-1}, 3503.5 cm^{-1}, 3515.6 cm^{-1} and 3516.4 cm^{-1}. The 3 main lines exhibited different polarization dependences corresponding to O-H bonds forming different angles to the crystallographic axes.

Heat treatments at 600-700°C in D_2O vapour atmosphere resulted in the appearance of OD^- lines at about 2587.1 cm^{-1}, 2596.6 cm^{-1} and 2600.4 cm^{-1} corresponding to the isotopic replica of the 3 main OH^- lines. The calculated anharmonicity parameters ($x_e \approx 0.0268$-0.0281) follow the general trend observed for hydroxyl ions in oxides [2]: the higher the harmonic vibrational frequency, the lower the anharmonicity.

The structure of OH^-/OD^- defect centres will be discussed on the basis of polarization and temperature dependent high resolution absorption spectra.

References

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