

Absorption Band at 1600 cm^{-1} in the IR Spectra of Irradiated MgO Crystals

Kvatchadze V* and Dekanozishvili G

E Andronikashvili Institute of Physics, I Javakhishvili Tbilisi State University, Tamarashvili street 6, 0186 Tbilisi, Georgia

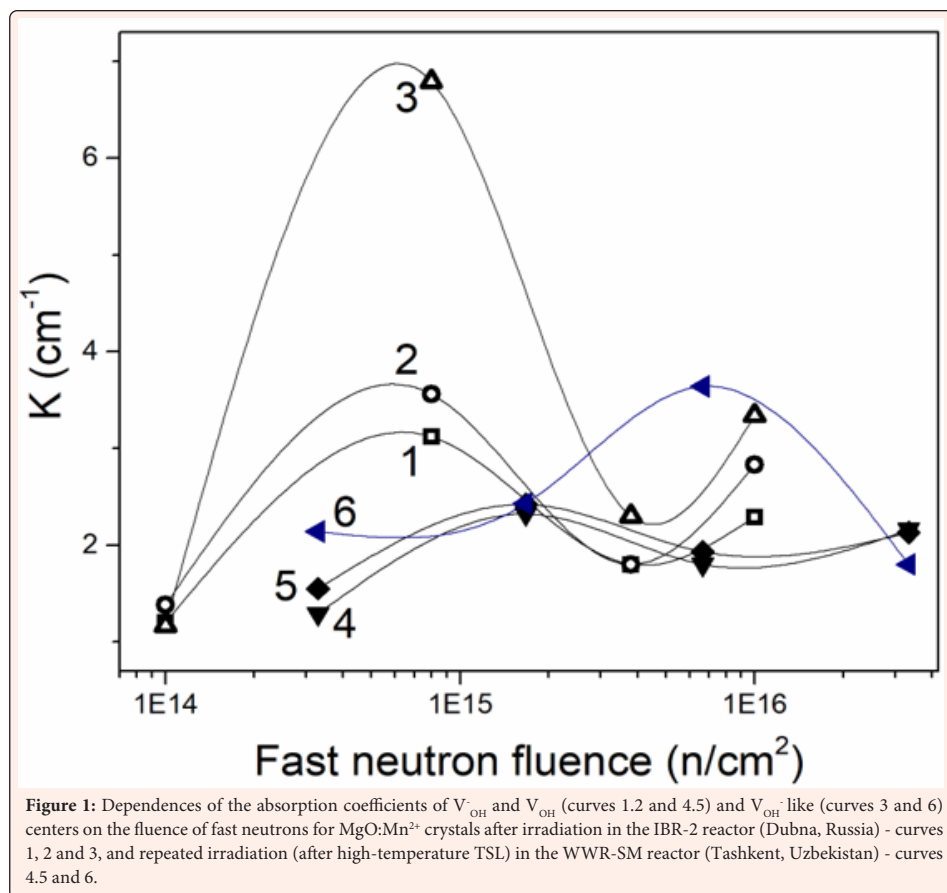
Abstract

In the IR spectra of nominally pure and doped MgO crystals after irradiation, an intense absorption band appears at 1600 cm^{-1} . This message discusses the model of the corresponding absorption center.

Opinion

The nature of OH⁻ ions and the products of their radiative decay (O²⁻ and H⁺) has been well studied for alkali halide crystals (LiF), which cannot be said about alkaline earth systems. Here we will consider the issue concerning the nature of the 1600 cm^{-1} band observed in the IR absorption spectra of magnesium oxide [1,2]. From the very beginning, it was attributed to impurity Ni ions [1]. However, based on the results obtained in [2], it was established that Ni ions must be excluded from further consideration, since in [2] paramagnetic Ni ions were not detected in any of the studied groups of crystals. It was also shown that the band at 1600 cm^{-1} appears only in combination with other bands (3290 cm^{-1} and 3370 cm^{-1}), which are due to stretching vibrations of OH⁻ groups: O²⁻-[Mg²⁺]-OH⁻ and OH⁻-[Mg²⁺]-OH⁻ (the so-called hole V_{OH}⁻ and V_{OH}⁺ centers) [2].

In contrast to these related bands, the exact model of the centers giving rise to the band at 1600 cm^{-1} has not been established. We assumed that this band can be attributed to hydroxyl-containing centers, since in many cases it behaves similarly to the bands at 3290 and 3370 cm^{-1} . Indeed, in [3] a correlation was established between the bands at 3290 cm^{-1} and 1600 cm^{-1} and later a linear relationship was discovered for these bands [4]. Thus, the centers responsible for the 1600 cm^{-1} band can be conditionally called V_{OH}⁻ like centers. This is, of course, not a complete solution to the problem. It is necessary to identify all the components of the model and their location. In this short message we kind of announce these studies. During research, there are often cases when all these centers (V_{OH}⁻ and V_{OH}⁺ on the one hand, and V_{OH}⁻ like centers on the other) exhibit the same behavior (please see the synchronous course of non-monotonic accumulation curves of these centers 1, 2 and 3 in Figure 1) and vice versa - when their effects are different (the maximum of curve 6 is located above the minimums of curves 4 and 5). Indeed, the linear interdependence of the related bands 3290 and 3370 cm^{-1} has a universal character [4].





It should also be noted the results obtained on samples after exposure to UV radiation (not yet published), which indicate the interconversion of the studied hole centers in a certain dose range ($V_{OH^{\cdot}}$ like $> < V_{OH^{\cdot}}$). This can partially explain the appearance of a maximum (curve 6 in Figure 1) above the minima of curves 4 and 5 (about 10^{16} n.cm⁻²). Regarding Figure 1, we also note the following. The hole center accumulation curves shown in Figure 1 are taken from [5]. There they serve other purposes and are not presented together like that. Here the picture is interesting in another respect. The positions of the maxima of the 1st set of graphs (1, 2 and 3) and the 2nd set (4 and 5, as well as the minimum of curve 6) practically coincide with each other, despite the fact that irradiation occurs in different reactors. (an interesting result for spectrometric methods of fast neutron dosimetry!). There is a shift, but it can be explained: after the 1st reactor irradiation, radiation structural defects were not removed from the sample. The difference in absolute values should be associated, for example, with higher irradiation temperatures under the conditions of reactor 2, etc.

References

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