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ELECTRONIC EXCITATIONS AND DEFECT CREATION IN WIDE-GAP MgO SINGLE CRYSTALS IRRADIATED WITH SWIFT HEAVY IONS

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Highly pure MgO single crystals are known as highly resistant to nonimpact mechanisms of Frenkel defect (FD) creation. One of the reasons is that the threshold energy of nonimpact FD creation in MgO is much higher than the band gap. So, the energy released at the recombination of a relaxed electron-hole (e-h) pair is insufficient for the defect creation. Furthermore, in MgO electrons, holes and excitons do not undergo transformation into a self-trapped state (see, e.g., [1]), which is an essential requirement for the relatively slow decay of electronic excitations (EE) into pairs of FD. However, as-grown or radiation-induced lattice defects and impurity ions may serve as traps for charge carriers, creating centres suitable for realisation of the nonimpact mechanism via the recombination of non-relaxed e-h pairs. The probability of such hot recombination is high under the conditions of high EE density, i.e. in the tracks of swift heavy ions, which transfer over 90% of their energy to electronic subsystem, unlike fast neutrons that create defects via direct knock-out (impact) mechanism.

A comparative study of radiation effects in Be²⁺-, Ca²⁺- and Al³⁺-doped MgO single crystals previously irradiated at 300 K with fast neutrons (1-2 MeV, fluence of 10¹⁶ n·cm⁻²) or with ²³⁸U ions (2.5 GeV, 10¹² ions·cm⁻²) has been performed in this study (see also [2]). It is shown that radiation-induced holes undergo localization nearby Ca²⁺, Be²⁺, bivalencies (v_cv_a) or Cr³⁺v_cCr³⁺ centers and form Coulomb recombination centers for both relaxed and hot holes. Hot e-h recombination is considered as one possible nonimpact mechanism of FD creation. The irradiated samples, in some cases subjected to uniaxial deformation of ~4% prior to irradiation, have been compared by measuring the thermally stimulated luminescence at 300–825 K through different optical filters. For thermochemically reduced (TCR) nominally pure MgO crystal, the excitation spectra for the emission of F (2.4 eV) and F⁺ centers (3.2 eV) as well as the reflection spectrum have been measured at 8 K using synchrotron radiation of 14–35 eV. For the same crystals, the spectra of steady cathodoluminescence (exciting electron energy of 5 keV, 6 K) have been measured as well. Typical emissions connected with the excitation of oxygen ions near cation (v_c) and anion (v_a) vacancies or v_cv_a have been detected in TCR and plastically deformed MgO as well as in ion-irradiated sample. So, the impact mechanism of defect creation induces stress and, consequently, formation of v_cv_a. A higher efficiency of FD creation in the samples deformed before ion-irradiation also confirms that the creation of these defects via hot recombination of carriers, one of which has undergone localization, is facilitated in ion-irradiated MgO. It was shown that highly mobile free excitons as well as e-h pairs efficiently interact with Cr³⁺ and Cr³⁺v_c centers causing the excitation of Cr³⁺ ions in MgO:Cr at 10 K (see also [3]).

References

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