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Charge trapping by iodine ions in photorefractive $Sn_2P_2S_6$ crystals

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ABSTRACT

Electron paramagnetic resonance (EPR) is used to establish the role of iodine as an electron trap in tin hypothiodiphosphate ($Sn_2P_2S_6$) crystals. Iodine ions are unintentionally incorporated when the crystals are grown by the chemical-vapor-transport method with SnI_4 as the transport agent. The $Sn_2P_2S_6$ crystals consist of Sn^{2+} ions and $(P_2S_6)^{4-}$ anionic groups. During growth, an iodine ion replaces a phosphorus in a few of the anionic groups, thus forming $(IPS_6)^{4-}$ molecular ions. Following an exposure at low temperature to 633 nm laser light, these $(IPS_6)^{4-}$ ions trap an electron and convert to EPR-active $(IPS_6)^{5-}$ groups with S = 1/2. A concentration near 1.1 × 10^{17} cm^{-3} is produced. The EPR spectrum from the $(IPS_6)^{5-}$ ions has well-resolved structure resulting from large hyperfine interactions with the ^{127}I and ^{31}P nuclei. Analysis of the angular dependence of the spectrum gives principal values of 1.9795, 2.0123, and 2.0581 for the *g* matrix, 232 MHz, 263 MHz, and 663 MHz for the ^{127}I hyperfine matrix, and 1507 MHz, 1803 MHz, and 1997 MHz for the ^{31}P hyperfine matrix. Results from quantum-chemistry modeling (unrestricted Hartree–Fock/second-order Møller–Plesset perturbation theory) support the $(IPS_6)^{5-}$ assignment for the EPR spectrum. The transient two-beam coupling gain can be improved in these photorefractive $Sn_2P_2S_6$ crystals by better controlling the point defects that trap charge.

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