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Charge trapping by iodine ions in photorefractive Sn₂P₂S₆ 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 (Sn₂P₂S₆) crystals. Iodine ions are unintentionally incorporated when the crystals are grown by the chemical-vapor-transport method with SnI₄ as the transport agent. The Sn₂P₂S₆ crystals consist of Sn²⁺ ions and (P₂S₆)⁴⁻ anionic groups. During growth, an iodine ion replaces a phosphorus in a few of the anionic groups, thus forming (IPS₆)⁴⁻ molecular ions. Following an exposure at low temperature to 633 nm laser light, these (IPS₆)⁴⁻ ions trap an electron and convert to EPR-active (IPS₆)⁵⁻ groups with S = 1/2. A concentration near 1.1 × 10¹⁷ cm⁻³ is produced. The EPR spectrum from the (IPS₆)⁵⁻ ions has well-resolved structure resulting from large hyperfine interactions with the ¹²⁷I and ³¹P 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 ¹²⁷I hyperfine matrix, and 1507 MHz, 1803 MHz, and 1997 MHz for the ³¹P hyperfine matrix. Results from quantum-chemistry modeling (unrestricted Hartree–Fock/second-order Møller–Plesset perturbation theory) support the (IPS₆)⁵⁻ assignment for the EPR spectrum. The transient two-beam coupling gain can be improved in these photorefractive Sn₂P₂S₆ crystals by better controlling the point defects that trap charge.

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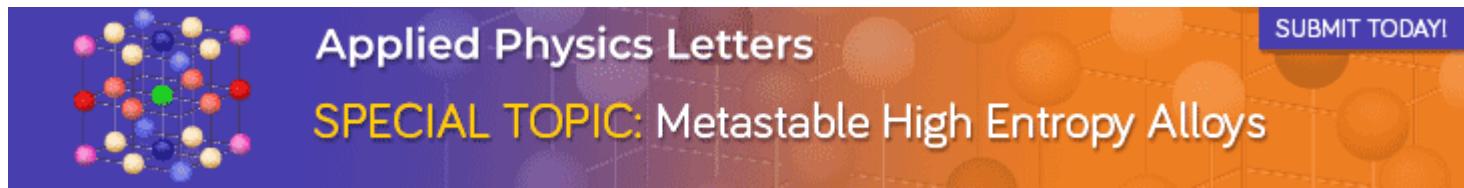
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