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Sulfur vacancies in photorefractive $Sn_2P_2S_6$ crystals

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ABSTRACT

A photoinduced electron paramagnetic resonance (EPR) spectrum in single crystals of $Sn_2P_2S_6$ (SPS) is assigned to an electron trapped at a sulfur vacancy. These vacancies are unintentionally present in undoped SPS crystals and are expected to play an important role in the photorefractive behavior of the material. Nonparamagnetic sulfur vacancies are formed during the initial growth of the crystal. Subsequent illumination below 100 K with 442 nm laser light easily converts these vacancies to EPR-active defects. The resulting S = 1/2 spectrum shows well-resolved and nearly isotropic hyperfine interactions with two P ions and two Sn ions. Partially resolved interactions with four additional neighboring Sn ions are also

with the corresponding principal axes along the *a*, *b*, and *c* directions in the crystal. The isotropic parts of the two primary ^{31}P hyperfine interactions are 19.5 and 32.6 MHz and the isotropic parts of the two primary Sn hyperfine interactions are 860 and 1320 MHz (the latter values are each an average for ^{117}Sn and ^{119}Sn). These hyperfine results suggest that singly ionized sulfur vacancies have a diffuse wave function in SPS crystals, and thus are shallow donors. Before illumination, sulfur vacancies are in the doubly ionized charge state because of compensation by unidentified acceptors. They then trap an electron during illumination. The EPR spectrum from the sulfur vacancy is destroyed when a crystal is heated above 120 K in the dark and reappears when the crystal is illuminated again at low temperature.

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