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Vacancy Defects in Photovoltaic Antimony Selenide

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Antimony selenide (Sb_2Se_3) is photovoltaic material with an optimal bandgap and a high optical absorption coefficient comprising of earth abundant elements. Solar cell power conversion efficiencies initially increased markedly but more recently the rate of increase has slowed. There is a large open circuit voltage consistent with the presence of detrimental concentrations of point defects. Here we report the results of variable energy positron annihilation lifetime measurements and related density functional theory calculations of positron lifetimes. Measurements have been performed on a series of closed-space sublimation deposited films and a range of single crystal samples including stochiometric with and without post-growth annealing, oxygen-doped and Sn-doped samples. The results provide evidence for the presence of both monovacancy and divacancy defects. The high implantation energy results from stoichiometric crystal grown from high purity stock and the CSS films subjected to a post-growth anneal exhibited spectra dominated by perfect lattice annihilations.

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