Mechanisms of carrier lifetime enhancement and conductivity-type switching on hydrogen-incorporated arsenic-doped $BaSi_2$

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Abstract: A comparative experimental and theoretical study of the role of H incorporation in As-doped $BaSi_2$ films has been carried out based on the experimental results that an optimal time of H treatment for the increase in photoresponsivity and carrier lifetime was in the range of 1 – 20 min. Adequate theoretical representation of the decay curves in the framework of the model for non-radiative processes accounted for various trap-related recombination mechanisms to estimate the trap concentration to be in the range of 1.9×10^{13} to 1.7×10^{14} cm^{-3}. Additionally, the extended theoretical ab initio quantum-chemical simulation of the electronic structure of the studied systems was performed. It was revealed that interstitial As atoms can mostly provide trap states in the gap while H atoms neutralize such traps. The experimentally observed unexpected switching in conductivity from n-type to p-type and vice versa in As-doped $BaSi_2$ with H incorporation was explained to specific configurations of point defects (an As impurity with a H atom in different positions and various interatomic As-H distances) which affect the position of states in the gap.

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