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Defect identification in semiconductors with positron annihilation: experiment and theory

FILIP TUOMISTO, Aalto University

Positron annihilation spectroscopy is a very powerful technique for the detection, identification and quantification of vacancy-type defects in semiconductors. In the past decades, it has been used to reveal the relationship between opto-electronic properties and specific defects in a wide variety of materials - examples include parasitic yellow luminescence in GaN, dominant acceptor defects in ZnO and broad-band absorption causing brown coloration in natural diamond. In typical binary compound semiconductors, the selective sensitivity of the technique is rather strongly limited to cation vacancies that possess significant open volume and suitable charge (negative of neutral). On the other hand, oxygen vacancies in oxide semiconductors are a widely debated topic. The properties attributed to oxygen vacancies include the inherent n-type conduction, poor p-type dopability, coloration (absorption), deep level luminescence and non-radiative recombination, while the only direct experimental evidence of their existence has been obtained on the crystal surface. We will present recent advances in combining state-of-the-art positron annihilation experiments and ab initio computational approaches. The latter can be used to model both the positron lifetime and the electron-positron momentum distribution - quantities that can be directly compared with experimental results. We have applied these methods to study vacancy-type defects in III-nitride semiconductors (GaN, AlN, InN) and oxides such as ZnO, SnO_2, In_2O_3 and Ga_2O_3. We will show that cation-vacancy-related defects are important compensating centers in all these materials when they are n-type. In addition, we will show that anion (N, O) vacancies can be detected when they appear as complexes with cation vacancies.