IDENTIFICATION OF VACANCY DEFECTS IN TRANSPARENT SEMICONDUCTING OXIDES: THE CASES OF ZnO, SnO_2 and In_2O_3

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Oxygen vacancies in oxide semiconductors have been a widely debated topic over the past decades. 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. However, direct experimental evidence of their existence is difficult to obtain.

Positron annihilation spectroscopy is a method sensitive to neutral and negatively charged open volume defects. The decreased electron density in a vacancy manifests itself as an increase of positron lifetime and the narrowing of the 511 keV photopeak in the annihilation γ spectrum, compared to a defect-free crystal. Positron lifetime spectroscopy provides information on the atomic structure, the charge state and often the concentration of the vacancies while the Doppler broadening of the photopeak allows the identification of atoms surrounding the vacancy defects. The combination of positron annihilation spectroscopy and supporting first-principles modeling of the measured annihilation parameters has been efficiently used to identify and quantify technologically important vacancy-related defects in, for example, group IV semiconductors, III-nitrides and ZnO [1].

We discuss our recent experimental and computational work on transparent semiconducting oxides and developments leading to the possibility of detecting oxygen vacancy-related defects in oxide semiconductors [2]. The examples cover materials systems such as ZnO and SnO_2 [3] as well as In_2O_3 [4]. We show that O vacancies may be directly detected in some of these oxides, in cases where they are complexed with cation vacancies. The detection is based on the modification of the positron annihilation signal of the cation vacancies when one or more oxygen vacancies are attached, similar as observed for nitrogen vacancies in InN [5].

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