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## Identification of the lattice vacancies in solids by means of electronpositron annihilation. Case studies for carbides, sulfides and oxides.

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A coincident measurement of the Doppler broadening of the positron-electron annihilation radiation is a powerful tool for the site detection of vacancies in complex substances. The coincident Doppler broadening of positron annihilation radiation (CDBPAR) gives an access to the electron momentum distribution of the core electrons of the atoms surrounding the annihilation site. In case of positron trapping at vacancies in ordered binary compounds this element-specific information allows for the identification of the sublattice on which the vacancies are located [1]. Due to the strong coupling of positron to defects the positron lifetime (PLT) technique allows the determination of the size and the dimensionality of free volume in which the positron is trapped [2]. High-precision measurements of a lattice constant by X-ray technique (HPX-ray) allow to follow the change of interatomic distances arising owing to interstitial type of defects [3].

The combination of Doppler broadening, positron lifetime, and X-ray data gives the unique information about the chemical and structural peculiarities of novel electronic materials on a nanoscale.

In this talk the recent results on vacancies identification in semiconducting, semimetallic, and metallic compounds, such as stoichiometric SiC, PbS, CdS as well as nonstoichiometric  $TiC_y$  and  $TiO_y$  will be presented. The methods by which the vacancies were introduced in above listed binary compounds were different, namely, low and high energy electron irradiation, sintering or chemical deposition.

The CDBPAR, PLT, and HPX-ray techniques are expected to be useful for an identification of defects when their origin is unclear as in as-grown, sintered or deposited paramagnetic, magnetic, dielectric, semiconducting, metallic or semimetallic compounds, for an atomic study of order-disorder processes in nonstoichiometric and amorphous materials, for a specific investigation of defects and atomic processes in complex condensed matter in general, etc.

[1] A. A. Rempel, W. Sprengel, H.-E. Schaefer et al, Phys.Rev.Letters 89, 185501 (2002).

- [2] A. A. Valeeva, A. A. Rempel, W. Sprengel, H.-E. Schaefer et al, PCCP 5, 2304 (2003).
- [3] C. Seitz, A. Rempel, A. Magerl, W. Sprengel, H.-E. Schaefer, MSF 433-436, 289 (2003)

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