

Exploring Hydrogen Storage Materials: Insights from Positron Annihilation Spectroscopy

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Positron annihilation spectroscopy (PAS) is a nondestructive technique used to characterize open volume defects in solids, such as vacancies, vacancy clusters, dislocations, and grain boundaries. Delocalized positrons probe the interstitial sites of the crystalline lattice. When a material contains open volume defects, positrons can be trapped there, allowing them to examine the local electron density and chemical environment of these defects. There are two key observables related to the positron annihilation process: the positron lifetime in the sample and the Doppler shift in the energy of annihilation gamma rays. Positron lifetime spectroscopy (PLS) can identify the types and concentrations of defects present in a sample, while coincidence Doppler broadening (CDB) provides information about the local chemical environment of those defects.

Hydrogen absorbed in solids occupies interstitial sites within the crystalline lattice, which are the same regions analyzed by delocalized positrons. Additionally, hydrogen is attracted to open volume defects and tends to segregate at the inner surfaces of these defects. Not only does hydrogen bind to existing open volume defects in the material, but its absorption also introduces new defects. The interaction between hydrogen and various defects, along with the defects created by hydrogen, can significantly impact hydrogen storage properties, including absorption capacity, reversibility, and the kinetics of hydrogen absorption and desorption. These phenomena can be thoroughly investigated using PAS. This will be illustrated in the following examples during the talk:

- (i) Hydrogen-induced vacancies in niobium
- (ii) Defects created by the formation and decomposition of metallic hydrides
- (iii) Characterization of lattice distortions in refractory metal high-entropy alloys and their relation to hydrogen absorption capacity.