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Hydrogen interaction with vacancies in Ti

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Titanium is an exothermic absorber of hydrogen. In the hydride phase Ti is able to absorb the hydrogen concentration as high as 1.4 wt.%. These properties make Ti and Ti-based alloys attractive for hydrogen storage applications. Hydrogen absorbed in Ti lattice may be trapped at open volume defects like vacancies, dislocations or grain boundaries. Hydrogen is not only trapped at existing defects but new defects can be also introduced by hydrogen loading. For these reasons it is very important to investigate interaction of hydrogen with defects in Ti.

In the present work hydrogen interaction with vacancies and vacancy-like defects in Ti was investigated employing positron lifetime spectroscopy combined with *ab-initio* theoretical modeling of vacancy hydrogen complexes.

Ab-initio modeling revealed that multiple hydrogen atoms can be trapped at vacancies in α-Ti lattice. In the lowest energy configuration hydrogen atoms are located close to the nearest neighbor tetrahedral sites around vacancy, see Fig. 1a. Lifetimes of positrons trapped at vacancies surrounded by various number of hydrogen atoms were calculated and are plotted in Fig. 1b. The equilibrium concentration of vacancy–hydrogen complexes has been calculated as well.

Positron lifetime measurement revealed that phase transition into the hydride phase is always accompanied by introduction of dislocations. Vacancies are created by hydrogen loading as well and agglomerate into small vacancy clusters. Absorbed hydrogen segregates at inner surfaces of these vacancy clusters.

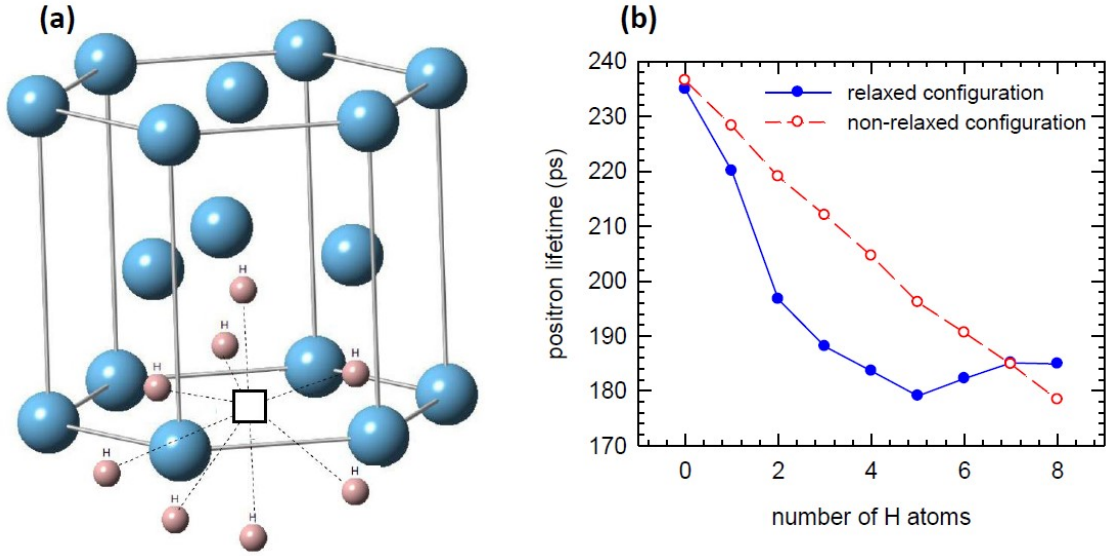

Fig.1. (a) Schematic depiction of a vacancy surrounded by 8 hydrogen atoms in the nearest neighbor tetrahedral sites; (b) calculated lifetimes of positrons trapped at vacancies surrounded by various numbers of hydrogen atoms.