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Vacancy dynamics and hydrogen retention in beryllium

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This contribution summarizes experimental and modeling studies of hydrogen retention in ion-implanted beryllium, focusing on the role of vacancy and self-interstitial atoms (SIA) dynamics during the implantation process. As the main modelling tool macroscopic rate equations (MRE) implemented in the CRDS code [1] and supported by density functional theory (DFT) calculations are used to simulate the dynamic behavior of irradiation induced defects along with hydrogen transport and trapping processes. The DFT data provide information on the energy landscape for hydrogen trapping and indicate that annihilation of irradiation induced vacancies and hydrogen-vacancy complexes with self-interstitial beryllium atoms occurs without an additional energy barrier, irrespective of the number of hydrogen atoms trapped in a vacancy. It also follows from DFT calculations that mobility of hydrogen-vacancy complexes can be neglected in MRE simulations. Effects of these assumptions are investigated in application to experimental conditions reported in [2], with a focus on the fluence dependence of the retained amount of hydrogen isotopes, including the experimentally observed saturation of retention at fluences above ~1022 m 2. Finally, an attempt is made to link the observed low temperature desorption stage to hydrogen release from cavities [3] formed by vacancy clustering.

[1] D. Matveev et al, Nucl. Instrum. Methods Phys. Res. B 430 (2018) 23
[2] M. Eichler et al, Nucl. Mater. Energy 19 (2019) 440
[3] M. Zibrov and K. Schmid, Nucl. Mater. Energy 30 (2022) 101121

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