O-6

Detection of defects and location of deuterium in displacement-damaged tungsten

Sabina Markelj[1], Esther Punzón-Quijorna[1], Mitja Kelemen[1], Thomas Schwarz-Selinger[2], Xin Jin[3], Eryang Lu[3], Flyura Djurabekova[3], Kai Nordlund[3], Janez Zavašnik[1], Andreja Šestan Zavašnik[1], Miguel L. Crespillo[4], Gaston García López[4], Rene Heller[5]

[1]Jožef Stefan Intitute, Slovenia
[2]Max-Planck-Institut fur Plasmaphysik, Germany
[3]University of Helsinki, Finland
[4]Center for Micro Analysis of Materials , Spain
[5]Helmholtz-Zentrum Dresden-Rossendorf , Germany

Due to its advantageous characteristics, tungsten (W) is the main plasma-facing material candidate for future fusion reactors. However, in a future nuclear environment, the W crystal lattice will be heavily altered due to defects caused by 14 MeV neutrons from the D-T fusion reaction, affecting the physical properties of the material. To examine defects created in the W lattice, we utilized Rutherford backscattering spectrometry in channeling configuration (RBS-C), a well-established method for studying lattice disorder and defect evolution induced by irradiation. To quantify the disorder, the change in the ion yield of light ions backscattered along a specific crystallographic direction is measured [1]. Moreover, when combining nuclear reaction analysis in channeling configuration (NRA-C) with RBS-C utilizing D(3He,p)4He nuclear reaction, we can gain insights into the location of trapped D in displacement-damaged W.

To study the defects and trapping of D, we irradiated W (111) and (100) single crystals (SC) with 10.8 MeV W ions at two different doses (0.02 and 0.2 dpa) and temperatures (300 and 800 K). Our goal was to create samples, with either dominantly single vacancies, small vacancy clusters or large vacancy clusters [2]. This was later on also confirmed by positron annihilation spectroscopy on our samples. The transmission electron microscopy (TEM) analysis of W (111) SC revealed dislocation lines and loops of different sizes, depending on the irradiation dose and temperature. Multi-energy RBS-C spectra analysis along the <111> direction unveiled distinct ion yield responses for each sample [3]. For the first time for W, we employed molecular dynamics (MD) simulations of overlapping cascades as input for the RBSADEC code [4], to simulate the RBS-C spectra. The simulated spectra agreed remarkably well with the experiment for the lower dose sample, but showed discrepancies for the high-dose-irradiated sample, attributed to the presence of large dislocation lines observed by TEM, which cannot be formed in finite-size MD cells [3]. New simulation results with larger MD cell and different MD potential for the high dose and high-temperature samples will be discussed.

Irradiated and with D plasma decorated W (100) SCs were used to perform NRA-C and RBS-C using a 0.8 MeV 3He probing beam and study the D location in the tungsten lattice. The maximum NRA signal was detected in the <100> axial and in the (110) planar channels [5]. The interpretation of the spectra with the RBSADEC code [4], recently upgraded to simulate the NRA-C signal, will also be discussed.

[1] Feldman et al., Academic Press, San Diego, (1982), pp. 88–116
[2] Hu et al. J. Nucl. Mater. 556, 153175 (2021)
[3] Markelj et al, Acta Materialia 263 (2024) 119499
[4] Zhang et al. Phys. Rev. E 94, 043319 (2016).
[5] Markelj et al. Nucl. Mater. Energ 39 (2024) 101630