Poster Session | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[PO-B2]Poster Session 2

Symposium B

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-13] Dynamics of Magnetism in Neutron Irradiated Iron-Chromium Steels

 $^{\circ}$ Jacob B. J. Chapman, Pui-Wai Ma, Sergei L. Dudarev (Culham Centre for Fusion Energy (CCFE), UK)

Ferritic-martensitic (F/M) steels, with a high chromium content, are critical materials for magnetic confinement fusion technology due to high temperature stability and corrosion resistance, facilitating the thermal efficiency necessary for fusion power plant operation. To predict the evolution of the steel microstructure and mechanical properties when subjected to sustained high doses of radiation at elevated temperatures, we must understand how radiation damage affects magnetic properties of the materials, which strongly influence phase stability and chromium solubility.

We investigate the effect of neutron irradiation on the magnetic properties of F/M steel alloys, relating experimentally observed [1] concentrations, radii and number densities of Cr precipitates within a Fe-Cr matrix to the dynamics and degradation/enhancement of magnetism across a broad range of temperatures. The Curie temperature is shown to vary, strongly dependent upon microstructure, increasing significantly with Cr precipitation observed at high doses and ageing times. These large-scale non-collinear calculations are performed using a method implementing magnetic cluster expansion (MCE), parameterised using a database of DFT-generated observables [2], with spin-dynamics (SD) incorporating both transverse and longitudinal spin fluctuations [3]. SD simulations provide valuable insight into the ageing of alloys under realistic magnetic confinement conditions to inform material choices and construction strategy for fusion power plant design.

This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

[1] E.R.Reese *et al.*, JNM **500**, 192 (2018); [2] M.Y.Lavrentiev *et al.*, JAP **109**, 07E123 (201); [3] P.-W.Ma *et al.*, PRB **81**, 184202 (2017)