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MULTI-SCALE MODELING OF INTERGRANULAR EMBRITTLEMENT IN TUNGSTEN ALLOYS

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Fusion power plant first wall and divertor systems represent one of the greatest materials challenges of all time. In the DEMO and commercial reactors the plasma facing materials will be exposed to totally unprecedented and unexplored irradiation conditions. The exposure to high-energy radiation (neutrons, helium and hydrogen) severely damages the microstructure of the materials by violently displacing atoms from their lattice and thereby creating voids, dislocation loops and bubbles consisting of helium and hydrogen. The resulting damage leads to hardening and embrittlement of the materials which ultimately leads to the failure of the first wall and divertor components. The most promosing candidate materials for such components are tungsten based alloys. At present, however, little is known about the interplay between radiation defects and the alloying elements and their effect on the hardening and embrittlement of the material. The proposed master thesis aims at directly contributing to the efforts of developing multi-scale computer models for the description of the plastic behaviour of tungsten based alloys under neutron irradiation, in the framework of the European Fusion Development Agreement (EFDA).

Goal The objective of the proposed work is to predict the plastic behaviour of polycrystalline tungsten alloys using the multi-scale modelling approach. The alloys will be selected based on the results of an ongoing computational screening of the properties of crystalline tungsten alloys (K. Lejaeghere). The following scheme will be followed; (i) First density functional theory (DFT) calculations are performed to characterize the properties of grain boundaries in W and W-based alloys. (ii) Secondly an interatomic potential is fitted to and benchmarked against the DFT derived database. (iii) The last stage consists of performing large-scale molecular dynamics (MD) simulations based on the derived interatomic potential to study the influence of alloying elements on the strength and fracture of grain boundaries.

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