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Modelling high dose irradiation damage in tungsten

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The realisation of economically viable fusion reactors requires the development of comprehensive materials models spanning the parameter space of simultaneous thermal, mechanical, and radiation loads. As materials data for such conditions is scarce, there is a clear benefit in simulating materials behaviour in silico from first principles: if we can accurately simulate how the microstructure in a metal evolves under irradiation, we may attempt to derive engineering-relevant properties from it.

Here, we present the molecular dynamics (MD) method as a powerful tool for generating high-dose irradiation microstructure in tungsten from first principles, predicting materials properties such as thermal conductivity [1], deuterium retention [2], lattice strains [3], and stress relaxation [4] consistent with experimental findings. We will discuss the principles, capabilities, and limitations of the method in reference to the aforementioned predictions, and list the steps involved in performing a typical irradiation damage simulation.

We demonstrate how MD can be used to build a virtual representation, or "digital shadow", of an experiment to predict the outcome before the actual experiment is performed [4]. While the scope of the fusion materials challenge is far broader than the examples presented here, we show that it is possible to derive predictions from first principles in a previously unexplored regime, and to validate them by a carefully tailored experiment.

[1] D.R. Mason et al., Phys. Rev. Mater 5.12, 125407 (2021)
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[3] D.R. Mason et al., PRL 125.22, 225503 (2020)
[4] A. Feichtmayer et al., Commun. Mater. 5.1, 218 (2024)