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TECHNOLOGY TRANSFER PROGRAMME

Simulations of microstructural changes induced by irradiation

The research group of the Applied Physics Department of the University of Alicante has significant expertise in modelling the radiation damage effects in structural materials used for fusion. More precisely, the team gathered existing information about cluster stabilities and mobilities together with the different models for growth of loops in Fe-based alloy under irradiation to better understand the damage caused to the microstructure and optimize future designs. This knowledge in kinetic Monte Carlo and molecular dynamics simulations could be used in other applications where materials are exposed to radiation: fusion and fission reactors, space, healthcare, ion implantation in the semiconductor industry.

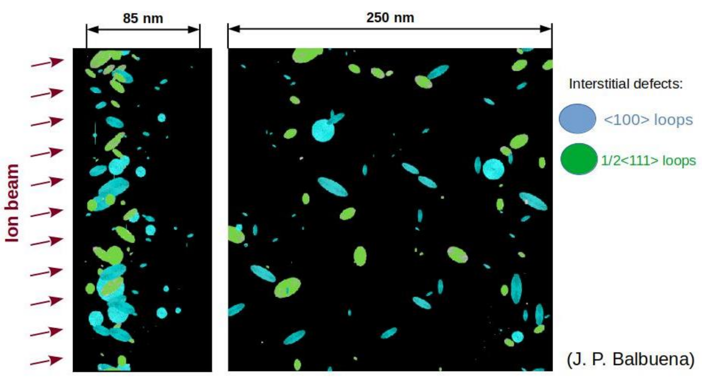
Description of the technology

University of Alicante researchers studied how loops nucleate and grow to understand the damage effects in Fe-based alloys under irradiation. It is well known that two types of loops are formed, <100> and ½<111>, and that the character, concentration, radius and sizes of these loops depend on the experimental conditions. However, the reason why both families of loops are observed is were not completely clear.

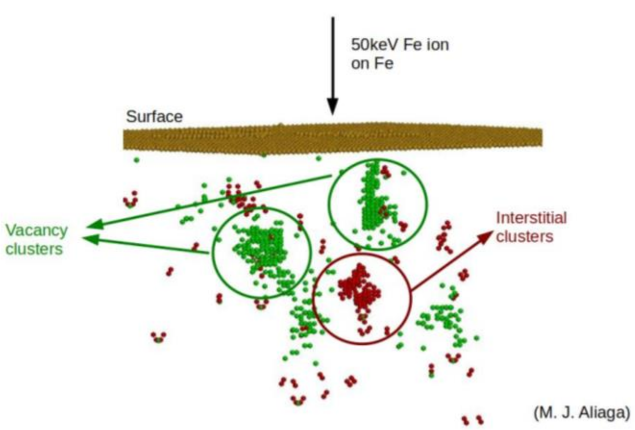
The know-how obtained is the microstructure evolution or loop growth in irradiated Fe, including the formation of both <100> and ½<111>, through kinetic Monte Carlo simulations and parameters obtained both from classical molecular dynamics simulations and density functional theory. The knowledge reported in the literature was used by the authors to define parameters and reactions to simulate irradiation at low energies, 100 keV, in Ultra High Pure Fe thin films at room temperature.

The study allows to explain how to simulate irradiation and thus, to understand the caused damage to the microstructure of Fe alloys and other materials.

Kinetic Monte Carlo calculations of Fe ion implantation in Fe



Damage produced by a 50 keV Fe ion in Fe: molecular dynamics simulations



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Innovation and advantages of the offer

The main benefit of this work and generated knowledge is to have gathered the existing information about cluster stabilities and mobilities together with the different models for growth of loops in Fe. This has contributed to develop a code which can be applied to the different fields requiring simulations of irradiation effects and microstructure evolution of Fe alloys.

Non-fusion Applications

The expertise of the researchers (Applied Physics and Materials) could be used to help in the development of models to understand damage produced by irradiation in materials for different applications, from fusion and fission reactors, to ion implantation in the semiconductor industry or the effects of radiation on materials in space.

EUROfusion Heritage

Supported by EUROfusion within the WP MAT IREMEV (Integrated Radiation Effects Modelling and Experimental Validation), the development of these codes and models was motivated by the search of optimal materials that can sustain the high levels of radiation that will be achieved in fusion reactors. This selection requires a basic understanding of damage production and damage evolution and to develop predictive models to understand which changes these materials will experience when exposed to radiation in a fusion reactor.

The models developed by the researchers are focused on understanding damage at an atomistic level and to try to develop predictive models for radiation effects under different conditions from ion irradiation to neutron damage. These simulations can be directly compared to experimental characterization techniques such as transmission electron microscopy (TEM) or positron annihilation spectroscopy (PAS).

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