Duc Nguyen-Manh, Materials Science and Nanotechnology

Magnetic and thermodynamic models of iron-based alloys for fusion materials application

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Developing predictive models for magnetic ferritic and ferritic martensitic steels that exhibit higher resistance to irradiation than the other steels and using mathematical modelling as an exploratory tool for possible alternative compositions and microstructures, require formulating control approximations and simplified algorithms for large-scale computer simulations. In this talk, we review how computational methods based on first-principles calculations can elucidate several key properties of iron-based alloys, encompassing phase stability at high temperatures, chemical bonding as well as the structures of defects formed under irradiation. Our study is part of broader programme of work aiming of finding out how the properties vary as a result of exposure to fusion neutron irradiation. First-principles methods based on electronic structure calculations provide reliable information about microscopic phenomena the understanding of which is required for the development of large-scale models, such as efficient tight-binding based many-body Stoner Hamiltonian, magnetic cluster expansion and spin-lattice dynamic simulations. These innovative developments in modelling techniques and high-performance parallelized computer platforms, as well improved experimental characterisation tools, will certainly provide powerful means for developing self-consistent approaches for validating materials performance in fusion power-plant environments. Very recently, our models have been extended to the investigation of new class of iron-based magnetic high-entropy alloys which are the potential candidates for fusion materials application due high swelling resistance properties under irradiation at high temperature.

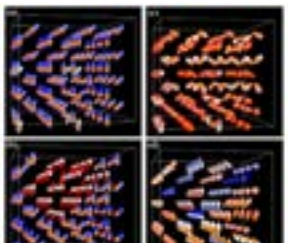

Figure 1: Constrained non-collinear Magnetic configurations in Fe-Cr alloys using combination of DFT and Monte-Carlo simulations for two different Cr concentrations: a) 6.25%, b)37.5% and their corresponding residual forces c), d), respectively. The grey and orange color denotes Cr and Fe atom, respectively.

Biography

Duc Nguyen-Manh is the Principal Investigator of Eurofusion program and working at the Culham Centre for Fusion Energy (UKAEA). Currently his interest and expertise are focused in modeling and computational materials science from first-principles models of radiation-induced phase transformations in engineering components for nuclear fusion power plants. The foundation of his research is based on multi-scale modelling concepts linking materials science with physics, chemistry and engineering application in order to reduce uncertainties in predicting complex phenomena. This scheme allows having a new understanding on the origin of ordering and segregation in Fe-based alloys from magnetic interactions via development of the new magnetic bond-order potentials and magnetic cluster expansion method.

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