

NOMATEN Hybrid Seminar

Location: NOMATEN seminar room

Time: 1 PM

gotomeeting room (for online): <https://meet.goto.com/NCBJmeetings/nomaten-seminar>

Seminar date: June 18th, 2024

Title: A novel approach for developing interatomic potentials in magnetic materials

Speaker name: Dr. Isaac Toda-Caraballo

Speaker affiliation: National Center from Metallurgical Research (CENIM) – Spanish National Research Council (CSIC)

Abstract: The use of atomistic simulations is extremely helpful in analysing the thermodynamics in metallic systems. DFT-based methods provide a powerful tool to describe phase stability, enthalpy and/or magnetic configurations, but are constrained to small systems due to a large computational cost. A proper treatment of the magnetic interactions is needed, since the magnetism is of paramount importance for the microstructural stability, especially in steels and high-entropy alloys containing magnetic elements. These magnetic interactions control the defects behaviour which affects the mechanical properties and the response under irradiation. Current interatomic potentials for molecular dynamics (MD) simulations still lack an adequate and general formulation to include magnetism into the simulations.

In this work, the universal equation of states (UES) is revisited and generalized by including ferromagnetic (FM) and antiferromagnetic (AFM) configurations with the aim of proposing a new formulation to develop interatomic potentials with magnetic contribution. A large database with around 120000 spin polarized density functional theory (DFT) calculated energies for different lattices, volumes, and magnetic moments for Fe, Ni, Co, Cr and Mn elements has been developed. This has allowed to propose a Generalized UES (GUES), which has been seen to correctly account for all DFT data generated, therefore paving the way to develop interatomic potentials with magnetic contribution. A first magnetic interatomic potential for the case of Fe is proposed and tested in other crystal lattices (A15 and C15), elastic constants, stresses in the lattice, vacancies, interstitials, forces at different temperatures, transformation paths between body-centered cubic, face-centered cubic, hexagonal close-packed, and simple cubic structures as well as γ -surfaces [1]. Additionally, the approximation has been now reformulated allowing for good predictions on non-collinear simulations, unifying in this way both ferromagnetic and antiferromagnetic configurations.

This work is performed in strong collaboration with J. S. Wróbel from the Faculty of Materials Science and Engineering (Warsaw University of Technology) and D. Nguyen-Manh from the Culham Centre for Fusion Energy (CCFE) - United Kingdom Atomic Energy Authority (UKAEA).

In addition to this, there will be an introduction of the research group and results concerning the development of new High Entropy Alloys for nuclear applications in the scope of the project INNUMAT, where both CENIM and NOMATEN participate and collaborate.

References

[1] I. Toda-Caraballo, J. S. Wróbel, D. Nguyen-Manh, Physical Review Materials 6, 043806 (2022)

Bio: Dr. Isaac Toda Caraballo is Tenured Scientist at the National Centre for Metallurgical Research (CENIM) of the Spanish National Research Council (CSIC). He studied Mathematics and Statistics, and finally obtained his PhD in Physics with a multiscale simulation to study the recrystallization and grain growth in ODS steels. After this, he joined the Department of Materials Science and Metallurgy of the University of Cambridge (UK) as a Research Associate for 6 years, where he started working in High Entropy Alloys developing physical based modelling for thermal stability and mechanical properties. He also performed research in fatigue in bearing steels and hydrogen embrittlement in austenitic steels, as well as some modelling mechanical properties in Mg-alloys and microstructural evolution in Al-alloys. After that he re-joined CENIM with a fellowship and finally got the permanent position as Tenured Scientist.

He works now in developing alloys for the energy industry. He is leading a national project on designing new alumina forming martensitic steels, and he is the PI of the Euratom project INNUMAT where he is developing new Alumina Forming reinforced High Entropy Alloys for the nuclear industry. He has recently created a new Digital and Simulation Laboratory in CENIM devoted to provide computational tools with relevant licenced thermodynamic software, machine learning and programming oriented to metallurgy. Additionally, he works also in Additive Manufacturing, participating in several projects in developing new compositions for AM, but also generating new meta-lattices for mechanical properties optimization.