

NOMATEN Hybrid Seminar

Location: NOMATEN seminar room

Time: 1 PM

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

Seminar date: March 19, 2024

Title: Microstructure stability of compositionally complex materials under extreme environment: Predictive modelling and experimental validation

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Abstract: Microstructural stability of multi-component systems under extreme environment represents one of most challenging issues not only in multi-scale materials modelling but also for developing reliable and advanced engineering components for nuclear material applications. Recently, compositionally complex alloys (CCAs) are designed as novel radiation-resistant materials for future fusion power plants while bcc-W based alloys including SMART (Selfpassivating Metallic Alloys with Reduced Thermal-oxidation) materials are developed at EUROfusion as a safety measure for plasma facing components in case of loss of coolant accident (LOCA). In addition, the microstructural evolution of the single-phase fcc-based CCAs under irradiation suggests that Fe-Cr-Ni-Mn high-entropy alloys are the promising material with potentially good corrosion resistance for nuclear fission systems.

To address these challenges, a new formulation of constrained thermodynamic formalism has been developed to model multi-component alloy system under irradiation for which point defects are being considered as the additional elements in the system [1]. The formalism is represented within matrix formulation via many-body cluster correlation functions which in turn can be computed efficiently from Monte-Carlo simulations in a combination with first principle-based cluster-expansion Hamiltonian. Applying the theory to bcc W-Ta-Cr-V-Hf systems [2], it is predicted that there is a strong enhancement of radiation induced stability in these quinary alloys as well as outstanding radiation resistance in the quaternary W-Ta-Cr-V system, For the latter case, the predictive modelling is an excellent agreement with observation of radiation-induced precipitates observed within Atom Probe Tomography analysis for the specific $W_{38}Ta_{36}Cr_{15}V_{11}$ alloy composition and irradiated temperature[3]. The similar modelling approach has been recently applied to study the composition stability at finite temperature for the magnetic fcc-based CCAs Fe-Cr-Ni-Mn [4] with a strong swelling resistance as well as for SMART self-passivating alloys W-Cr-Y=Zr as structural materials in DEMO fusion reactors [5]. Finally, I will address some new results from atomistic modelling in predicting microstructure for Tritium retention and permeation in W and its oxides that have an important implication in predicting the important issue of detritiation for the maintenance of fusion engineering material components under waste-treating environment or in accident scenarios.

References

[1] D. Nguyen-Manh et al., Phys. Rev. Mater., 5, 065401 (2021).

[2] O. El-Atwani et al., Sci. Adv. 5, 2002 (2019); Nature Communications, 14, 2516 (2023).

- [3] D. Sobieraj et al., *Physical Chemistry Chemical Physics*, 22, 23929 (2020).
[4] M. Fedorov et al., *Phys. Rev. B*, 101, 174416 (2020); *Acta Mater.*, 255, 119047 (2023). [5]
D. Sobieraj et al., *Metals*, 11, 743 (2021); *JAMS*, 2, 100011 (2023).
[6] M. Christensen et al., *Nucl. Mater. Energy*, 38, 101611, (2024).

Bio: Dr. Duc Nguyen-Manh is a distinguished Senior Research Scientist at the UK Atomic Energy Authority's Culham Centre for Fusion Energy and an Academic Visiting Fellow at the University of Oxford's Department of Materials. With a career starting in 1987, Dr. Nguyen-Manh's expertise spans nuclear materials, multiscale materials modeling, and high-performance computing. His deep knowledge in DFT-based large-scale atomistic simulations, statistical methods in physics, interatomic potentials development for MD simulations, elasticity theory, and neutronic simulations highlights his proficiency in multiscale material modeling. Holding a Ph.D. in Physics from CNRS Grenoble, France, he has contributed significantly to the field, collaborating extensively with European and international partners within EUROfusion MAT/IREMEV and MAT/HHFM WorkPackages. This collaboration is evidenced by his impressive H-index of 45 and over 250 publications in prestigious journals. His work has greatly advanced the understanding of materials under irradiation, earning him a prominent position in international collaborations and scientific advisory boards.