Direction des énergies
Service de Recherches de Métallurgie Physique
Commissariat à l'énergie atomique et aux énergies alternatives

Post-doctoral position at SRMP, Université Paris-Saclay, CEA

A one year (with a possible extension to 2 years) post-doctoral position is open at Service de Recherches de Métallurgie Physique (SRMP), Université Paris-Saclay, CEA, France, starting from november 2021 - early 2022. The post-doctoral fellow will join a collaborative project "SYNERGY-AI" that brings together atomic-scale theoretical and experimental methods together with Artificial Intelligence (AI) [1-3]. The project is funded by the program "Numerical Simulations" of CEA.

Scientific context and goals

Present-day materials science enables simulations and experimental observations of defect nucleation, recombination, migration and transition at the atomic scale. However, their accurate interpretation implies a challenge. The most prevalent approaches for atomic-scale identification and interpretation of microstructure produced in simulations or experiments, like Atom Probe Tomography (APT), are currently based on rather heuristic methods that rely on the parameters chosen by the user. Such interpretation is very laborious, non-universal and subjective, as it depends on the user's choice of parameters. Therefore, the development of universal and robust tools for structural analysis is indispensable.

The goal of the SYNERGY-AI project is to develop novel Machine Learning (ML) and/or Deep Learning (DL) protocols for the structural analysis, which will rely on mathematical statistics in conjunction with theoretical physical knowledge.

Required skills

We are looking for a motivated candidate with PhD in materials science, physics or related discipline, skilled in programming with Python and Fortran. Previous experience in identification of defects in crystalline solids from atomic-scale simulations/experiments or experience in usage of ML/DL protocols is a plus.

How to apply

Please send your application including a motivation letter and complete CV with the references that we may contact to Alexandra Goryaeva (alexandra.goryaeva@cea.fr) and Mihai-Cosmin Marinica (mihai-cosmin.marinica@cea.fr).

References

[1] A. M. Goryaeva, C. Lapointe, C. Dai, J.-B. Maillet, M.-C. Marinica, (2020). Reinforcing materials modelling by encoding the structures of defects in crystalline solids into distortion scores. *Nature Communications*, **11**, 4691

[2] A. M. Goryaeva, J-B. Maillet, M.-C. Marinica (2019). Towards better efficiency of interatomic linear machine learning potentials. *Computational Materials Science*, **166**, 200-209

[3] K. Arakawa, M.-C. Marinica, S. Fitzgerald, L. Proville, D. Nguyen-Manh, S. L. Dudarev, P.-W. Ma, T. D. Swinburne, A. M. Goryaeva, T. Yamada, T. Amino, S. Arai, Y. Yamamoto, K. Higuchi, N. Tanaka, H. Yasuda, T. Yasuda, H. Mori (2020) Quantum De-trapping and Transport of Heavy Defects in Tungsten. *Nature Materials*, **19**, 508-511