12-month renewable post-doc position at SRMP, CEA/Saclay, France

Title: **Automatic machine learning identification of nanoscale features in transmission electron microscopy images**

Key-words: **Machine learning, High entropy alloys, TEM**

Research area: **Solid State Physics, Materials Science**

Summary of the Project:

Imaging nanoscale features using transmission electron microscopy (TEM) is key to predicting and assessing the mechanical behaviour of structural materials in nuclear reactors or in the fields of nanotechnology. These features, visible by phase contrast (nanobubbles) or diffraction contrast (dislocation loops or coherent precipitates), are prime candidates for automation. Analysing these micrographs manually is often tedious, time-consuming, non-universal and somehow subjective.

In this project, the objective is to develop a Python-based framework for data treatment of transmission electron microscopy (TEM) images.
Machine Learning approaches will be implemented in order to tackle the following tasks:
- Data collection: The success of any machine learning approach is linked to the database quality. In this project, a huge database is available. Four microscopists are involved in the project and will continuously enrich the database with images containing easily recognizable features.
- Denoising and finding the defect contour both through existing open-access software and in-house developed descriptors. Representative ROI (region-of-Interest) will be generated on images.
- Design of the Convolutional Neural Network (CNN) Architecture and model training: A collective feature map will be generated for the entire images in order to identify some representatives ROI. Each ROI is then overlaid to the original feature map and is passed to the CNN for individual region classifications. Secondly, recent advances in image segmentation will be placed in the core engine of the workflow.
- Model performance metrics: The aim is to reach a compromise between the training time and the detector performance.

The process will be applied to nanometer-sized features formed under irradiation in nuclear oriented materials (Co-free high entropy alloys (HEA), UO2, storage materials) and precipitates in materials with a technological interest (coherent Cr precipitates in Cu or SiC precipitates in Al). An example of the process applied to a HEA is given in the figure below.

Funding: The project is funded by the program “Numerical Simulations” of CEA.

Qualifications: Applicants must hold a Ph.D. degree in Solid State Physics, Materials Science or in a closely related area. Previous experience in Python or Fortran programming or usage of ML/DL protocols will be appreciated.

Practical information: The Service de Recherches de Métallurgie Physique (SRMP) is part of the Department of Materials for Nuclear energy at CEA-Saclay. It is located 20 km south-west of Paris, in the area called Plateau de Saclay. The SRMP research laboratory has 30 full-time members with 25 graduate students.

Collaboration : CEA Saclay (DES/ISAS/DMN/SRMP) ; CEA Grenoble (DRT/LITEN/DTNM/STDC/LCAE) ; CEA Cadarache (DES/IRESNE/DEC/SA3E/LCPC) and CNRS (ICMPE - UMR 7182 - CNRS – UPEC)

Time frame: 1 year: January 2022 / December 2022, renewable 1 year

How to apply: Candidates must return a motivation letter, CV, and contact information of two references to Estelle Meslin (estelle.meslin@cea.fr) and Alexandra Goryaeva (alexandra.goryaeva@cea.fr)

References:

[1] M. Nastar, L.T. Belkacemi, E. Meslin, M. Loyer-Prost, Thermodynamic model for lattice point defect-mediated semi-coherent precipitation in alloys, Communications Materials. 2 (2021) 1–11.
[2] A. Bhattacharya, J. Henry, B. Décamps, S.J. Zinkle, E. Meslin, Helium causing disappearance of a/2<111> dislocation loops in binary Fe-Cr ferritic alloys, Journal of Nuclear Materials. 556 (2021) 153213.

[3] A.M. Goryaeva, C. Lapointe, C. Dai, J. Dérès, J.-B. Maillet, M.-C. Marinica, Reinforcing materials modelling by encoding the structures of defects in crystalline solids into distortion scores, Nat Commun. 11 (2020) 4691.
[4] L.T. Belkacemi, E. Meslin, B. Décamps, B. Radiguet, J. Henry, Radiation-induced bcc-fcc phase transformation in a Fe-3%Ni alloy, Acta Materialia. (2018).

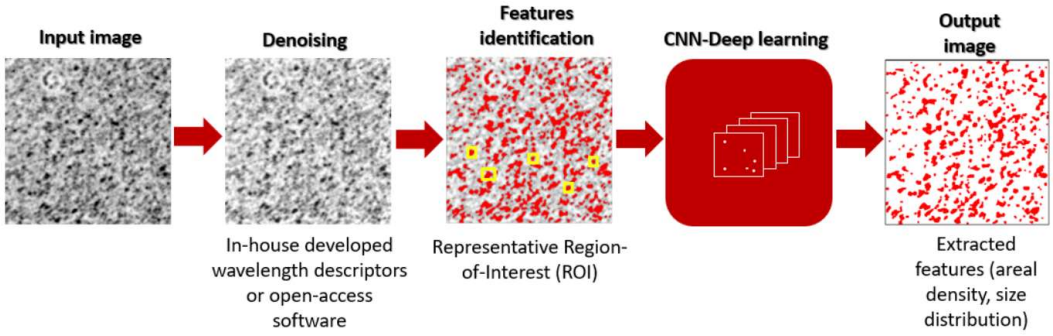

Illustration of the methodology using CNN detectors applied to an inverse WBDF image presenting dots-shaped dislocation loops formed in a Co-free HEA irradiated with 2 MeV Fe ions at liquid nitrogen temperature.