Phase-field modelling of grain boundaries at equilibrium and under irradiation

Yanis Calbert[1], Ludovic Thuinet[1], and Luca Messina[2]

[1]*Univ. Lille, CNRS, INRAE, Centrale Lille Institut, UMR 8207, UMET, Unité Matériaux et Transformations, F-59000, Lille, France*
[2]*CEA, DEs, IRESNE, DEC-Service d'Études et de Simulation du Comportement des Combustibles, Cadarache F-13108 Saint-Paul-Lez-Durance, France*

Metallic alloys used in nuclear power plants are under permanent irradiation which causes fast modification of their microstructure through a large variety of defects interacting with each other: interstitials, vacancies, point defect clusters, dislocations, grain boundaries (GBs), etc. In particular, segregation of atoms in these conditions can be observed at GBs, which can alter the structural integrity of the materials. Despite the numerous improvements achieved so far to understand radiation-induced segregation (RIS) at GBs through cutting-edge experimental or modelling tools, several observations remain unexplained. This might be due to the huge diversity of GB structures and the resulting difficulty to correctly describe their interactions with solute and point defect (PD) diffusion.

Recently, phase-field (PF) approaches have been developed to predict RIS behaviour in binary alloys for different conditions. However, in their formalism, the description of GB was still basic since the thermodynamic and elastic properties of the GB and the bulk phase were supposed to be the same, the GB being treated as a simple absorbing plane for PDs ("planar sink" model). As a consequence, these approaches fail to predict thermal segregation, which may interplay with RIS resulting in complex segregation profile at GBs. On the other side, defect generation due to irradiation is often given at constant rate for vacancies and interstitials in PF modelling, however, other phenomena occur such as ballistic damage, displacement cascade, etc.

To overcome the limitations of this "planar sink" model, we first propose in this work to better describe the thermodynamic and elasticity heterogeneities between the bulk phase and the GB. For this purpose, a density-based model recently proposed in the literature is adopted, allowing to recover the well documented "W-shape" segregation profile observed experimentally under irradiation. Secondly, we propose ballistic damage and cascade displacement generation method implementations to our PF model. Case studies will be presented on Fe−Cr and nickel base model alloys for nuclear applications.