ICAMS[2]

INTERDISCIPLINARY COLLOQUIUM ON ADVANCED MATERIALS SIMULATION

COLLOQUIUM

Invited Talk, Tuesday, May 7, 2:00 p.m. - 2:40 p.m., ICAMS[2] session: **T3**

A coupled diffusion-phase field-crystal plasticity framework to study grain boundary cavitation in irradiated materials

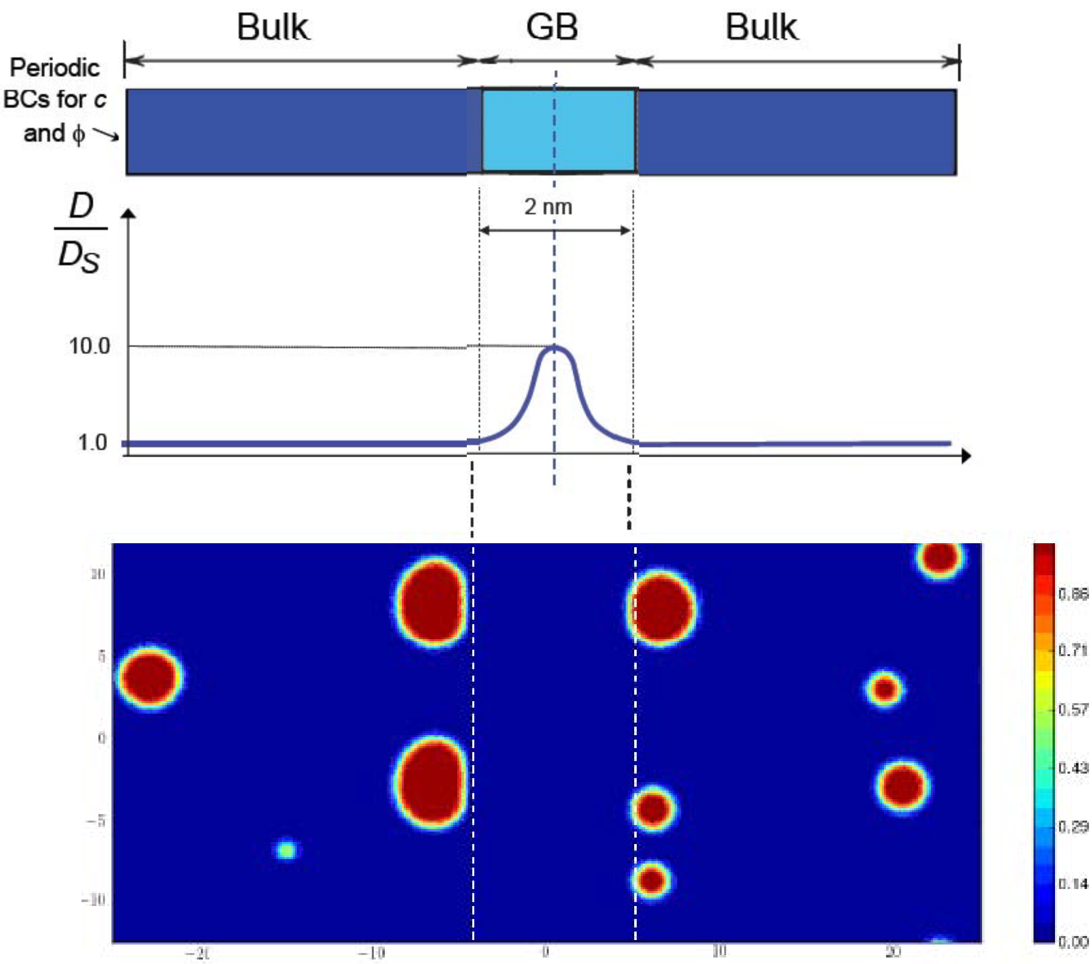
Aurélien Villani†, Samuel Forest† and Benoit Appolaire††, Esteban P. Busso†

†Centre des Matériaux, Ecole des Mines de Paris CNRS UMR 7633, BP 87, 91003 Evry Cedex,
‡LEM, ONERA, CNRS UMR 104, BP 72, 92322 Châtillon, FRANCE

Some of the most deleterious degradation mechanisms in high temperature polycrystalline materials are those caused by the diffusion of point defects (i.e. vacancies or interstitial atoms) through either the crystal lattice or the grain boundary regions, and by their interaction with other lattice defects such as dislocations and grain boundaries. They can lead to cavitation, local swelling, creep, hardening and embrittlement due to the formation of point defect clusters, amongst others. A detailed physical understanding of experimental observations and measurements of point defect production, diffusion, and trapping requires appropriate theoretical and modelling tools to study the complex phenomena involved.

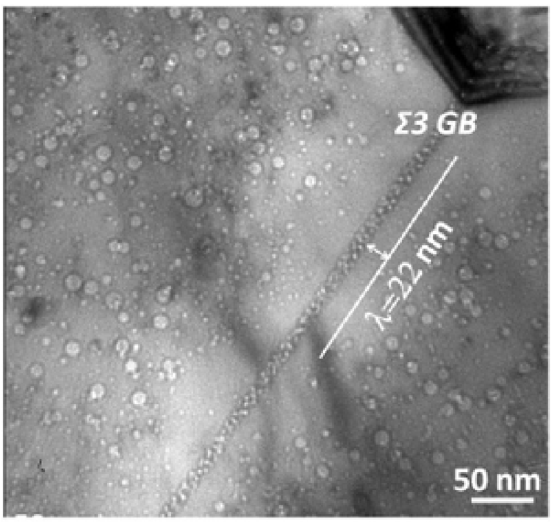
In the present work, the coupling between vacancy diffusion and stress is first considered by investigating a pressure driven vacancy diffusion mechanism in an elasto-visco-plastic polycrystalline material. A suitable form for the stress dependent isotropic diffusion flux is expressed in terms of the vacancy concentration, the main chemical potential gradient and the mechanical coupling, with the latter being expressed in terms of the trace of the stress tensor. Since inelastic strain is known to be mainly produced by dislocation glide and the rate of slip is controlled by dislocation climb, the effect of the local level of vacancy concentration is accounted for on the rate of slip in the coupled diffusion-crystal plasticity continuum framework. The framework is implemented into the finite element method and a parametric study is conducted on a polycrystal aggregate to study the influence of microstructural variables (e.g. dislocation density, grain size) and stress on the diffusion phenomena.

The coalescence of vacancy clusters into stable grain boundary cavities is then investigated. Such type of cavities are at the origin of the damage seen in irradiated materials and in bimaterial interfaces exposed to uneven atomic fluxes (i.e. Kirkendall effect), where the role of the local stress triaxiality is crucial. To that purpose, phase field techniques are relied upon to extend the diffusion-crystal plasticity framework to incorporate a non-convex free energy potential. The coupled framework is then used to study the effect of visco-plasticity at the grain level and vacancy diffusion in the grain and grain boundary regions on the growth behaviour of grain boundary cavities.



(a)

Predicted development of void (stable vacancy cluster) free and void rich zones at and adjacent to a grain boundary (GB) obtained with the coupled diffusion-stress-phase field framework.



(b)

The phenomenon has also been observed experimentally, as shown by the radiation-induced voids in (b) near an asymmetric tilt GB in irradiated Cu (Han et al., Acta Mat., 2012). In the model, the GB has been introduced as a diffuse region with a greater vacancy diffusivity than that in the bulk (DGB=10 Ds)