Modelling of degradation and reliability of crystalline materials

PROJECT DETAILS

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PROJECT DESCRIPTION

Radiation damage is known to lead to materials failure and thus is of critical importance to lifetime and safety within nuclear reactors. While materials mechanical behavior under irradiation has been subject to numerous studies, the current predictive capabilities appear limited. Observations and physical models have shown that the most important damage contributions arise from point defect localization –leading to void swelling- and creep.

It was recently found that void swelling can be prevented via use of non coherent heterophase interfaces. It is very likely that other interface types may exhibit similar trends. Unfortunately, no tool is available to generally predict the effect of interface composition (monophase, heterophase) and structure (geometry, roughness) on its propensity to resist radiation damage (both via defect localization and creep). These limitations motivate the proposed study which aims at developing such tool. Given the multi-scale multi physics nature of the problem, the consortium is formed by experts in the fields of materials modeling via ab initio, molecular dynamics and continuum modeling as well as of materials characterization and processing via mechanical alloying and physical vapor deposition. The program aims at constructing a bottom-up framework allowing discovery and quantifications of materials damage mechanisms and effects on mechanical properties for novel crystalline materials with large interfacial areas. Model validation will arise through direct comparison with materials testing for a wide array of materials systems (metal/metal, metal/oxide, oxide/oxyde).

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