Thesis defence Mohamed EL BAKOURI

In silico approach to model and characterize radiation-induced microstructural changes in materials - Fe and Ni as test cases

Abstract:

Ion beams are widely used in numerous fields for fundamental research or technical applications that include electro-optical devices, engineered nanostructures, strain engineering, nuclear materials, and space exploration. Ion beams are indeed a powerful tool to synthesize, shape, test, or modify the properties of materials. In most cases, the desired goals are enabled by the energy transfer from the energetic particles to atomic nuclei as well as electrons of the target, but energy deposition usually leads to defect generation and associated undesired damage accumulation. Therefore, understanding the mechanisms of defect formation and evolution in materials appears to be a crucial task.

Damage accumulation in irradiated materials is commonly studied through a phenomenological analysis of parameters such as the elastic strain or the disordering fraction that can be obtained via experimental characterization techniques, namely Rutherford backscattering spectrometry in channeling mode (RBS/C) and X-ray diffraction (XRD). Although these parameters convey information regarding lattice displacements in the materials, establishing a connection with the actual defect structure and density is not straightforward, and neither is the quantitative comparison with a modeling study at any scale. For this purpose, it is required to both develop ad hoc computational tools to calculate (pseudo-like experimental) signals from modeling data and determine basic information regarding typical defects as 'seen' by those techniques or as inherent to the defects.

This thesis addresses these two issues, dealing with Fe and Ni as test cases. First, a full computational methodology is proposed in order to produce model, single-crystal-like objects containing a single defect type of varying density or size, that are used to determine basic defect information such as their relaxation volume and their disordering efficiency by means of RBS/C or XRD signal simulations. These two computed quantities can be used to interpret strain and disorder levels derived from experimental RBS/C or XRD signals, exploit modeling data, and feed multiscale computational codes simulating radiation damage. Second, RBS/C and XRD signals are generated based on molecular dynamics (MD) atomic-scale data mimicking a prolonged irradiation time to derive disorder and strain kinetics; we show that it is possible to define various steps in the microstructural changes, each one being attributable to well-identified defect structures, as these latter are known from the analysis of the MD data. This computationally derived information can then be used to interpret experimental disordering kinetics.