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Combining experimental and computational approaches for the understanding of the basic mechanisms of irradiation-defect formation and evolution

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Ion beams are currently used in numerous fields of material science. It is crucial to have powerful tools to characterize irradiated materials and to have a better understanding of the basic mechanisms of the ion/solid interactions through mastering the technical aspects of the use of ion beams.

The aim of the thesis work is to develop new approaches that combine experimental characterization techniques, such as high-resolution X-Ray Diffraction (XRD) and ion channeling with computational methods such as molecular dynamics and rate equation cluster dynamic, to study the generation process of defects and damage in irradiated materials. The method will mainly rely on the cross-checking between experimental and computational irradiation data and between XRD and ion channeling characterization techniques.

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