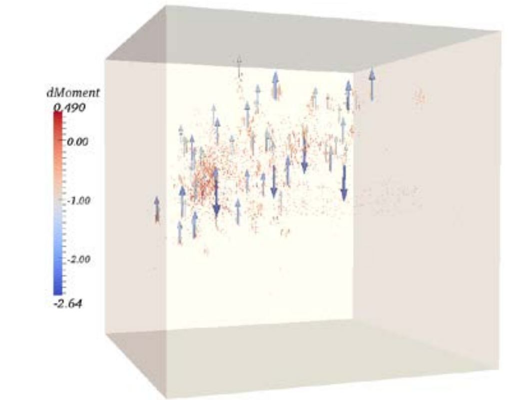
**Center for Defect Physics in Structural Materials (CDP)**
**EFRC Director: G. Malcolm Stocks**
**Lead Institution: Oak Ridge National Laboratory**

***Mission Statement:*** *To enhance our fundamental understanding of the defects, defect interactions, and defect dynamics that determine the performance of structural materials in extreme environments.*

**Coarse Graining Approach to Large Scale *Ab Initio (DFT)* Calculations**

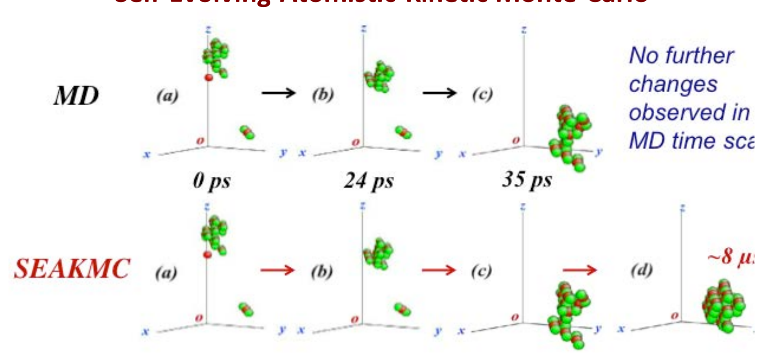



*Changes in local magnetic moments on Fe atoms during a 50KeV radiation damage cascade – 1,024,000 atom supercell: blue (red) moment reduction (enhancement)*

Defects of various types are ubiquitous in structural materials and ultimately control their properties. When materials are exposed to irradiation, the existing defects are altered and new ones created. Consequently, the properties of materials under irradiation continually evolve in response to defect creation, defect annihilation, and resulting changes in microstructure. The *Energy Frontier Center for Defect Physics in Structural Materials (CDP)* is developing an unprecedented level of knowledge about defect physics at the finest temporal and spatial scales in irradiated materials through the development and use of new computational and experimental tools to access these scales. Through a focus on Fe and Fe-based alloys as models of the steels that are the workhorse structural materials for energy, the knowledge derived from CDP activities will provide the requisite foundation to accurately predict how materials respond and perform under irradiation, while simultaneously laying the groundwork to guide and accelerate the development of materials that are resistant to radiation-induced property changes.

The CDP employs a multidisciplinary team that is developing and deploying novel experimental (X-ray, Transmission Electron Microscopy (TEM), Nano-mechanical testing) and theoretical techniques (large scale *ab initio* electronic structure, quantum informed molecular dynamics, atomistic kinetic Monte-Carlo methods) that can jointly probe the production and evolution of irradiation induced defects, their subsequent interaction with dislocations and consequent effect on materials strength. Specifically, the CDP develops approaches that *push the length and timescales of experiment down* and the *length and timescales of theory modeling and simulation up* to a point where they overlap; thereby, allowing the most direct tests of the underlying theoretical models. This approach makes it possible, for the first time, to directly test models and to identify strengths and deficiencies and to develop models that have

**Self-Evolving-Atomistic-Kinetic Monte-Carlo**



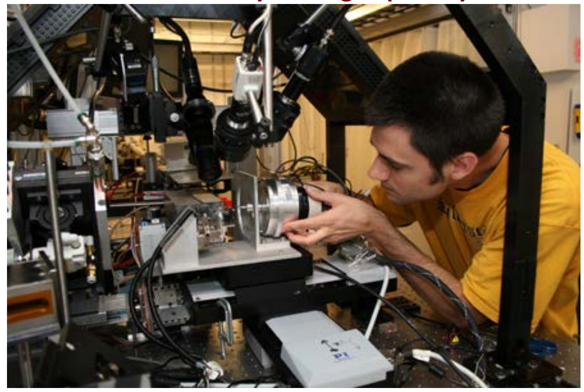

***SEAKMC:*** *A new atomistic approach to modeling defect diffusion/interaction at time scales ($10^{-7}$ – $10^{3}$ s) inaccessible to Molecular Dynamics (< $10^{-6}$ s)* been validated at the most basic level of “atoms and electrons”.

Within this overall context the CDP focuses on two interconnected themes:

- *Defect formation and short-term evolution under irradiation*
- *Dislocation interactions with radiation produced defects*

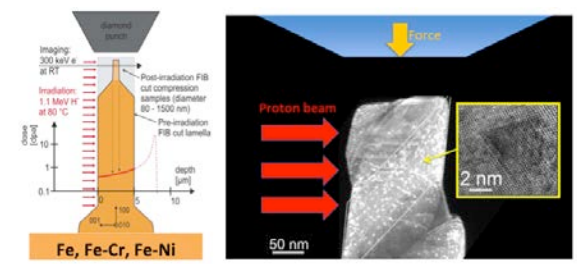
In the first theme, the goal is to obtain a quantitative understanding of the mechanisms of defect formation and short-term defect evolution that determine material behavior and the properties of Fe-based alloys under irradiation. We employ advanced *ab initio* and atomistic methods to determine defect character and properties, and the influence of magnetism and solutes. In addition we directly compare predicted microstructures to experimental results obtained by employing x-ray diffuse scattering and *in situ* TEM. The goal of the second theme is to develop a rigorous understanding of the fundamental unit events that control strength and deformation by studying the interaction of dislocations with both preexisting defects, such as grain boundaries, and the defects produced by irradiation. To accomplish this, the CDP is deploying a suite of new experimental tools that includes: 3D X-ray microscopy, TEM (both high resolution and *in situ* deformation) and *in situ* nano-mechanical testing.

**New In Situ 3D X-ray Testing Capability at APS**



*Sub-micron stress measurement by 3D X-ray*

**Nano-Mechanical Testing of Irradiated Pillars**




*Quantitative in situ mechanical testing of irradiated samples during transmission microscopy provides direct information on defect interactions and effects on plastic deformation.*

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