

Center for Defect Physics in Structural Materials (CDP)

www.ms.ornl.gov/cdp/index.shtml

Goal

Provide a fundamental understanding of materials defects, defect interactions, and defect dynamics, thereby enabling atomistic control and manipulation of defects and the charting of new pathways to the development of improved materials with ultrahigh strength, toughness, and radiation resistance.

Partner Institutions

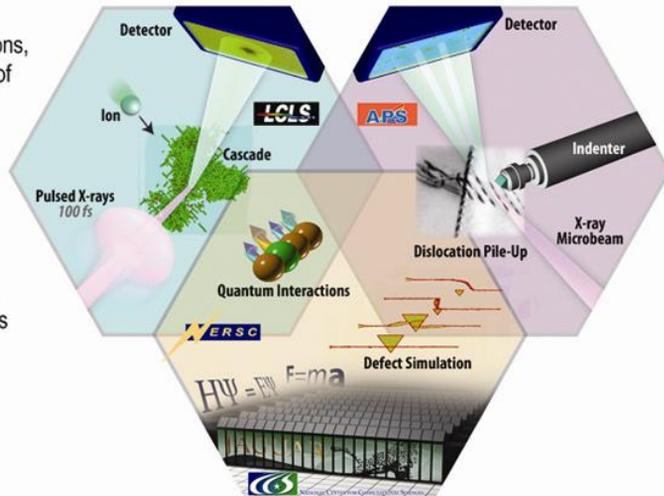


Approach

Deploy first-of-its-kind measurements and *ab initio* quantum calculations of the structure, interactions, and dynamics of defects in structural materials

Interrelated Thrust Areas

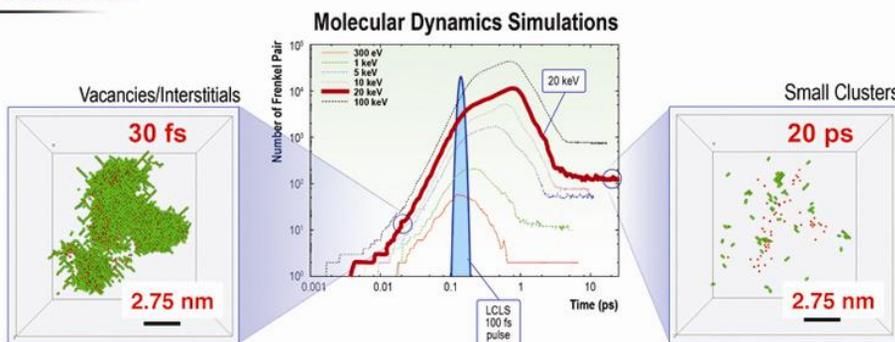
- Fundamental physics of defect formation and evolution during irradiation
- Fundamental physics of defect interactions during deformation
- Quantum theory of defects and interactions



Defect Production During Irradiation

Primary damage formation

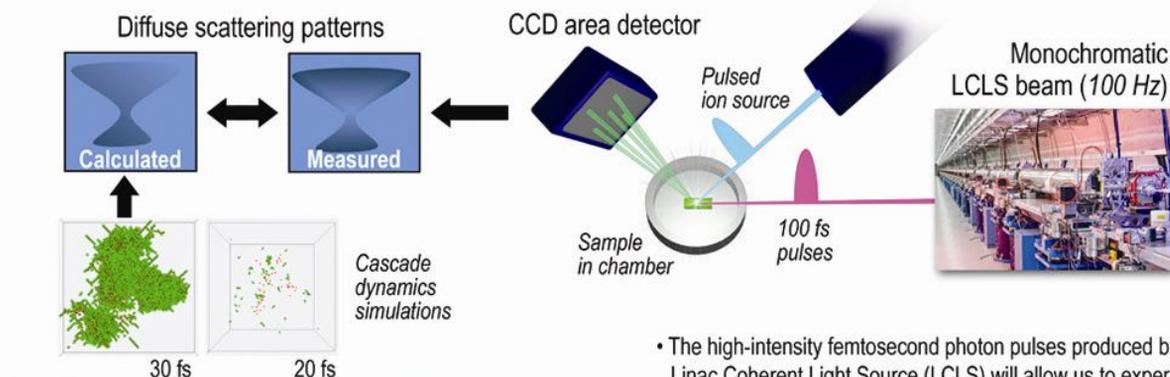
- Essentially everything that is known about primary damage formation comes from classical molecular dynamics (MD) simulations
- The first few picoseconds set the stage



Molecular dynamics simulations of displacement cascade evolution have spanned 50 years

Experimental measurements of cascade dynamics and evolution will be possible for the first time with sub-picosecond X-ray pulses

Sub-picosecond Cascade Dynamics Evolution Investigation



- The high-intensity femtosecond photon pulses produced by the Linac Coherent Light Source (LCLS) will allow us to experimentally study picosecond cascade dynamics
- High-performance computing and advanced modeling will allow us to relate experimental results to cascade dynamics

