INL/CON-24-81021

Atomistic Modeling of Irradiation-Induced Defects and Clusters in Additively-Manufactured Austenitic Stainless Steel

OCTOBER 2024

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http://www.inl.gov

Prepared for the
U.S. Department of Energy
Office of Nuclear Energy
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517

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About the Presenter

- Mathew Swisher, Idaho National Laboratory
  - PhD in Mechanical Engineering and Computation
  - Atomistic Scale Modeling
    - Irradiation induced defects and defect clusters
    - Nanoscale Solid-Liquid-Gas Interfaces
- AMMT: Radiation Damage Modeling Group
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  - Sourabh Kadambi
  - W. Tanner Yorgason
  - Andrea Jokisaari

This work was funded by the Advanced Materials and Manufacturing Technologies program, which is supported by the Office of Nuclear Energy of the U.S. Department of Energy. This research made use of the resources of the High Performance Computing Center at Idaho National Laboratory, which is supported by the Office of Nuclear Energy of the U.S. Department of Energy and the Nuclear Science User Facilities under Contract No. DE-AC07-05ID14517.

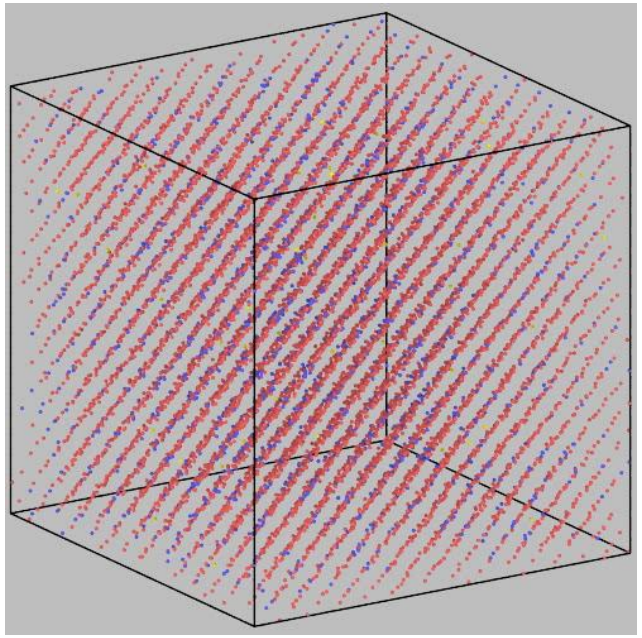
Problem Statement

- Understand the behavior of irradiation induced defects at an atomistic level using more realistic molecular dynamics (MD) models of alloys that are more representative of 316 stainless steel
  - Limited amount of atomistic scale data available for irradiation induced defects in austenitic stainless steels

- Need a more detailed understanding of how the solute composition of AM-316 SS may affect the generation of point defects and growth rate of defect clusters
  - Investigate effect of variation in composition due to powder feedstock and/or additive manufacturing
  - Adapt existing modeling techniques developed for single element systems to alloys
  - Determine which mechanisms are most significant (focusing on carbon content)

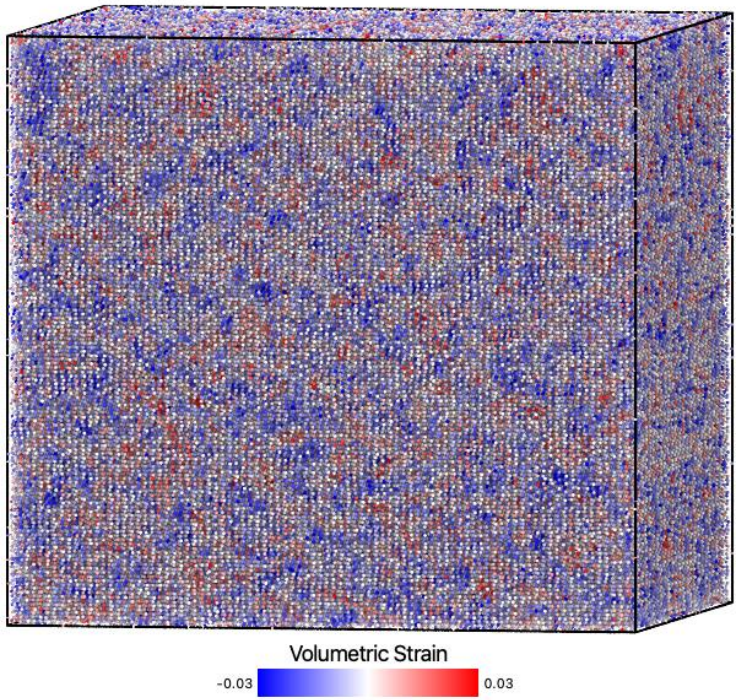
Background: Molecular Dynamics

- Each atom is tracked through time using Newtonian physics
  - Forces acting on each atom are calculated using a potential energy model
- Utilizing a preexisting “off the shelf” model commonly used to model steels
  - Fe-Cr-C (ABOP), Henriksson et al, 2013
  - Combined with a ZBL potential, for close range interactions
- Base model generated from randomizing elements on an FCC lattice structure
  - Carbon atoms inserted at octahedra sites



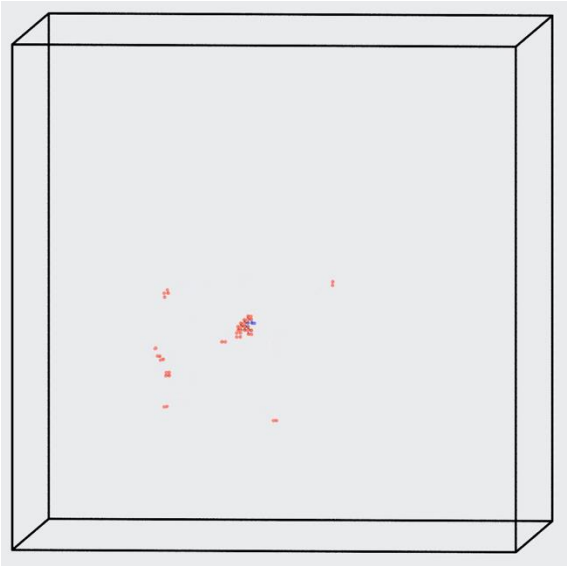
Challenges of modeling alloys

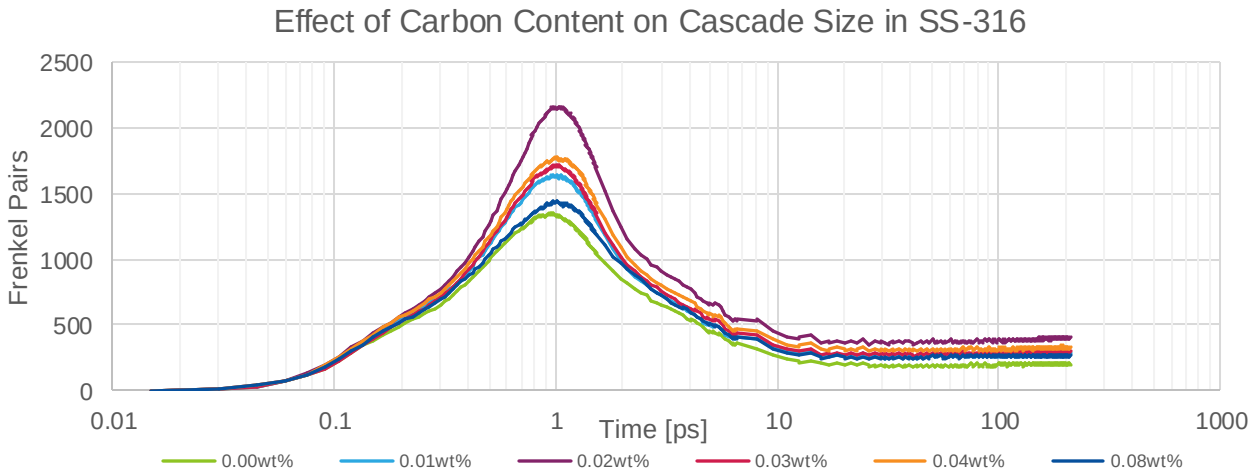
- Need to model a randomized mixture of elements
  - Requires more complex potential energy model
  - Base alloy model inherently contains significant variations in stress/strain
    - Variation in stress can be larger than the effects we would like to measure
  - Dimensionality of problem is dependent on the permutation of elemental configurations
- Generally best methodology for high dimensional problems is Monte Carlo
  - Converges $\boldsymbol{O}\left(\sqrt{\boldsymbol{n}}\right)$, but not effected by dimensionality
  - Need to replicate many simulations with new randomizations to average across all possible local configurations of elements



Primary Radiation Damage

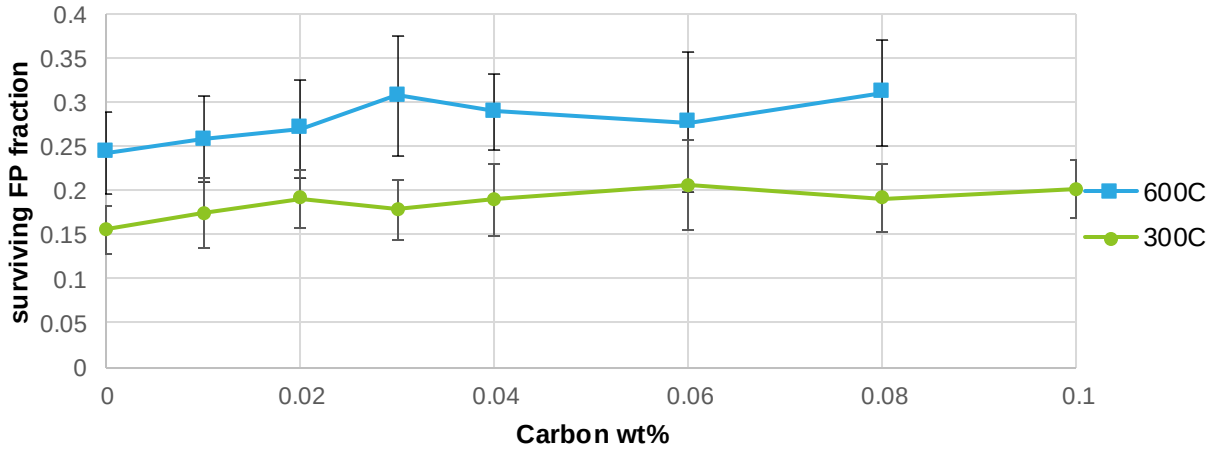
- Use MD to model collision cascades of various energies
  - Kinetic Energy: 15 keV
  - Temperature: 300C, 600C
  - Use frictional model to represent electron stopping
  - Track number occupancy of lattice sites to track the number of point defects
- Need to replicate cascade simulations with varying initial PKA directions and starting configurations

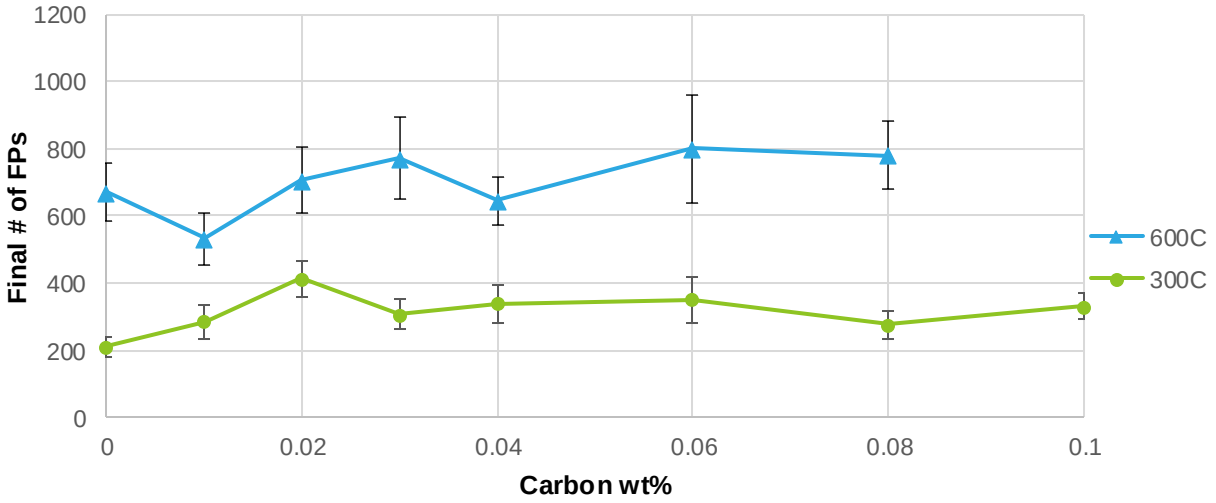




Primary Radiation Damage

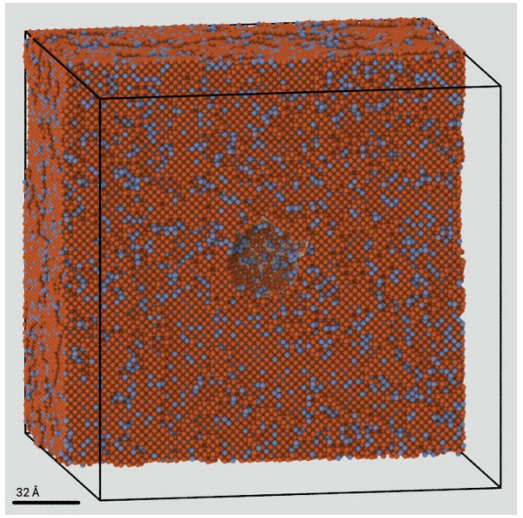
- Significant measurement noise even using 20 replicas for each condition
- Higher temperatures result in a more point defects being generated and a higher fraction of defects surviving recombination
- Carbon content corresponds with increasing rate of defects created from 0.00 to 0.02 wt%
  - Carbon percentage in 316 is generally higher than this range

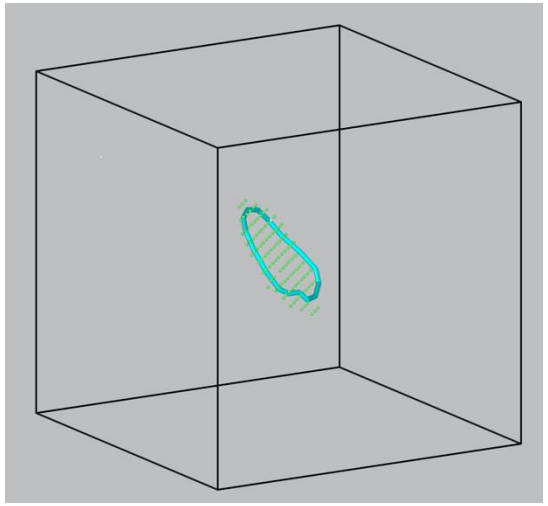


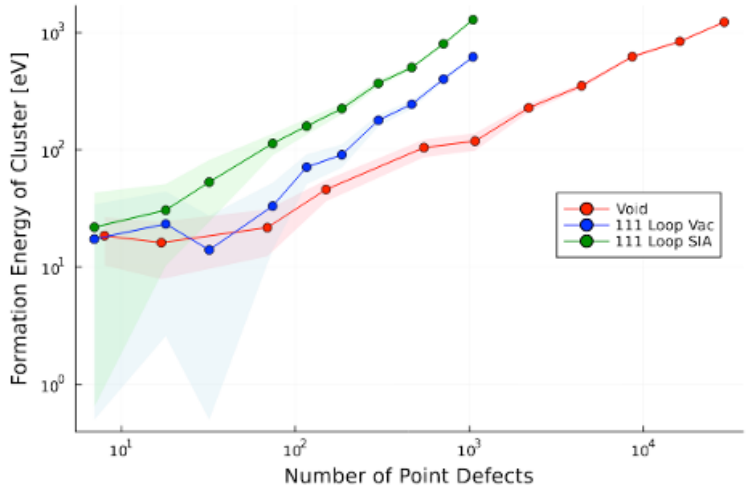


Defect Cluster Formation Energies

- FE of defect clusters is an important parameter for cluster dynamics modeling
- Utilize MD to compare the energy of a given arrangement of atoms w/wo defect cluster inserted
  - Every datapoint is 200-500 simulations
- Local variation in material composition only has a small effect on average cluster energy since each cluster interacts with many atoms
  - More significant for clusters of <20 defects

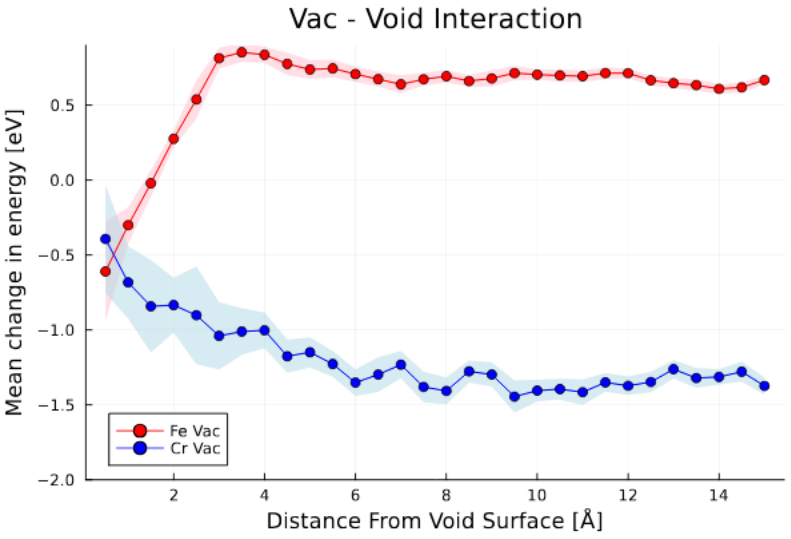


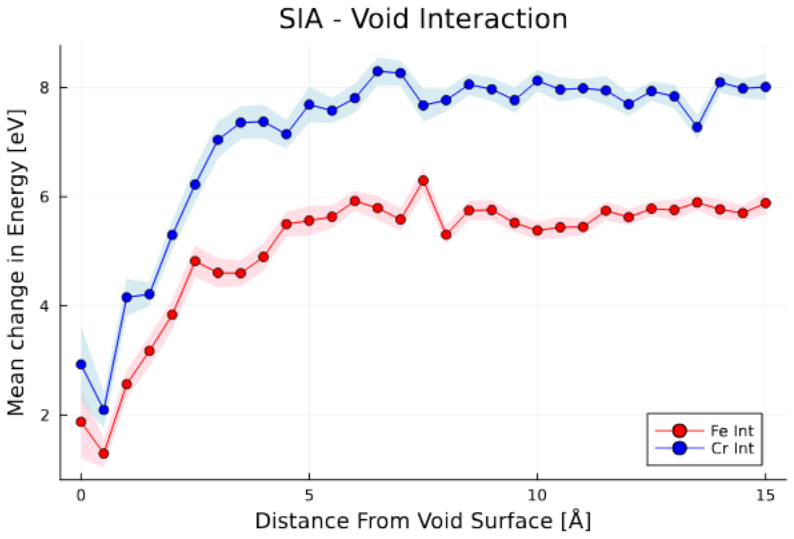




Point Defect – Void Interactions

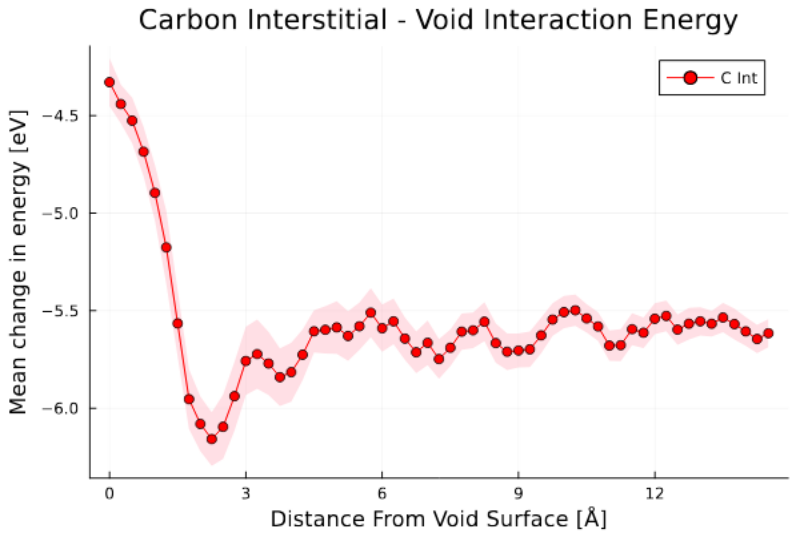
- Additional measurements needed to measure the sink efficiency of defect clusters, using methodology developed by Kohnert et al (2017)
- Measurements taken by creating a set of 20 voids in randomized FCC lattices and allowing the structure to equilibrate 300C, before minimizing structure energy
- Randomly place defects at different distances from the void surfaces, minimize the structure energy, and take measurement
- Capture distance determined by a $\Delta E = -k_b T$
  - Proportional to sink efficiency

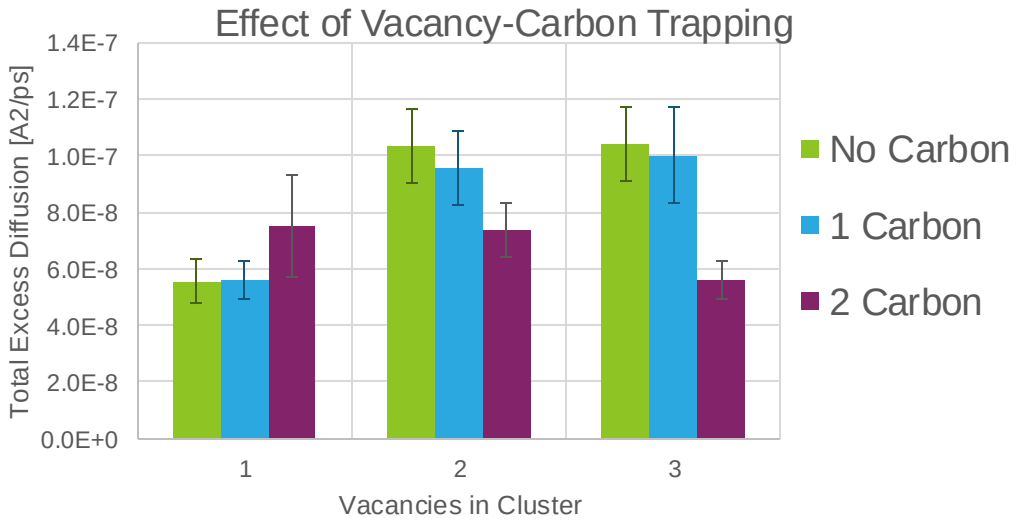




Carbon - Void Interaction

- This simulation technique can also be used to investigate the interaction between carbon interstitials and voids
- Unlike in the previous interactions with voids, we can see that there is a strong energy well 2.5 Å from the void surface
- This suggest that interactions between carbon atoms and voids could inhibit the transport of groups of vacancies
  - Mechanism has been shown in ferritic steels (carbon-vacancy trapping)
- Additional diffusional MD simulations were performed verify that this mechanism may function with very small clusters





Summary and Conclusions

- Adapting existing atomistic techniques for measuring the behavior of irradiation induced defects in austenitic alloys
- Built out datasets needed to begin parameterizing cluster dynamics to model the growth of defect clusters
- Investigated how the component elements interact with irradiation induced defects
- Shown that the carbon-vacancy trapping mechanism is a possible explanation for why increased carbon content in 316SS reduces growth rate of voids

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