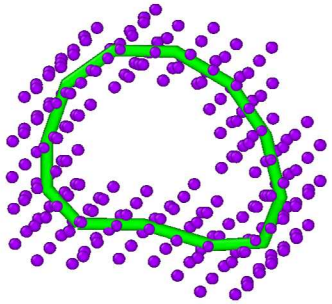
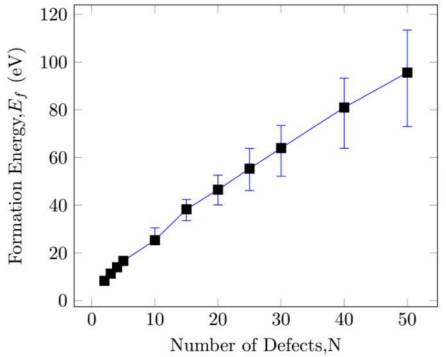
SAND2019-2991C

Georgia Tech Mechanical Engineering
The George W. Woodruff School of Mechanical Engineering

Sandia National Laboratories

Defect Characterization in bcc Nb





$$E_F = a_o\sqrt{N_{SIA}}ln(N_{SIA}) - a_1\sqrt{N_{SIA}} + a_2$$

Presented by

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U.S. DEPARTMENT OF ENERGY

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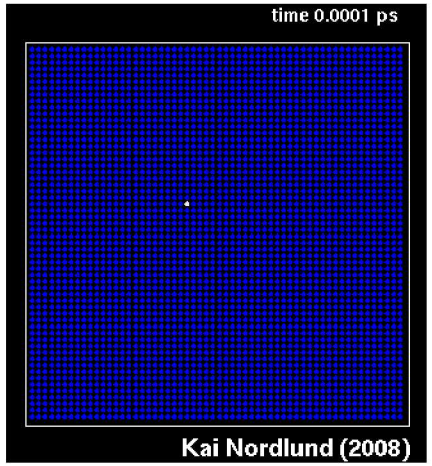
Outline

1. Radiation induced defects in metals
2. Modeling of defect clusters
3. Trends in formation and binding energies of defect clusters
4. Statistical characterization of SIA defects
5. Conclusion

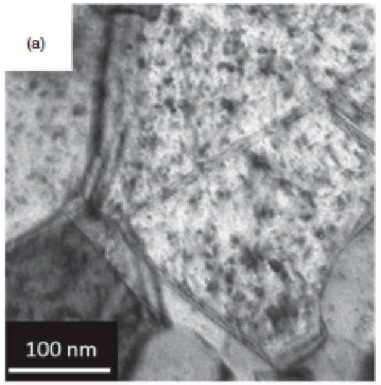
Radiation Damage and Aging

Picoseconds — Microseconds - Days — Seconds - Years

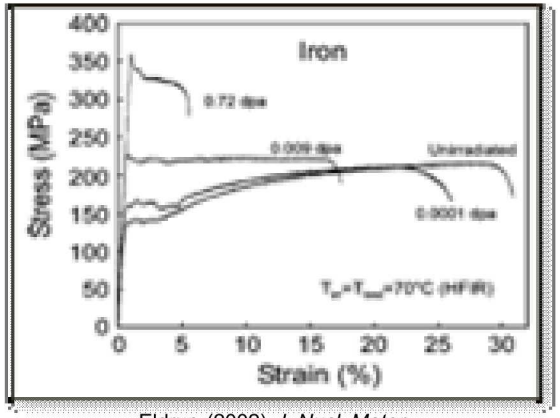
Tens of nm — Hundreds of nm - Hundreds of μm — cm - m



Nordlund (2008)



Muntifering et al. (2015) *Mater Res Lett.*



Eldrup (2002) *J. Nucl. Mater.*

"Special" Physics

- keV-energy collision between nuclei
- Energy loss to electronic excitation
- Transition to high P-T
- Long term relaxation

Radiation Damage

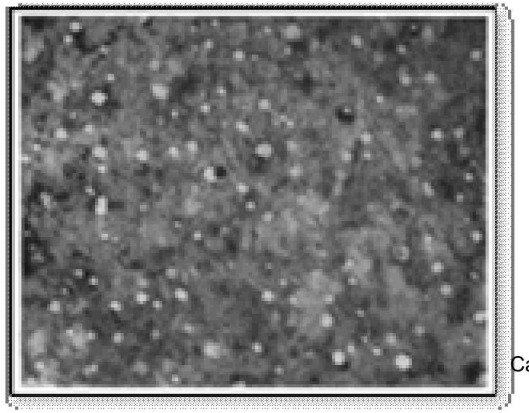
- Defect production: Frenkel pairs, Cascade
- Transmutation
- Segregation
- Amorphization
- Sputtering

Radiation Effects

- Hardening
- Swelling
- Embrittlement

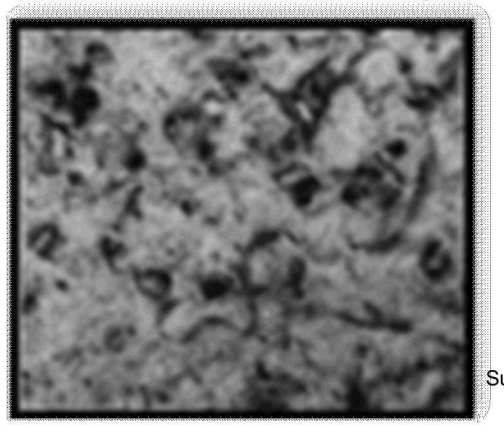
Common Radiation-Induced Defects

Voids



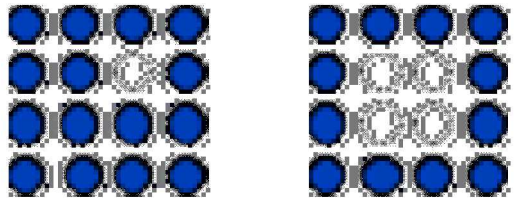
Cawrhorne and Fulton (1967)

Dislocation loops

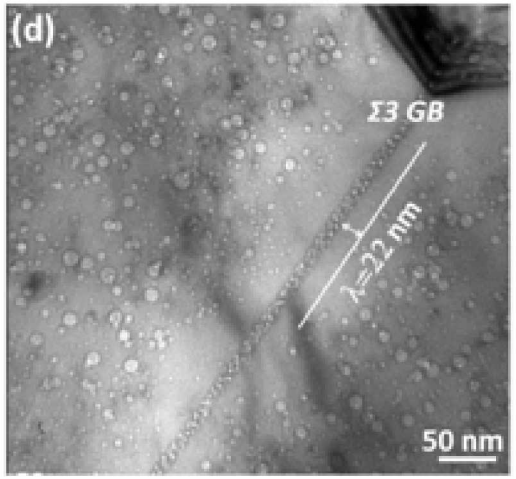


Sugano et al. (2004)

Vacancies

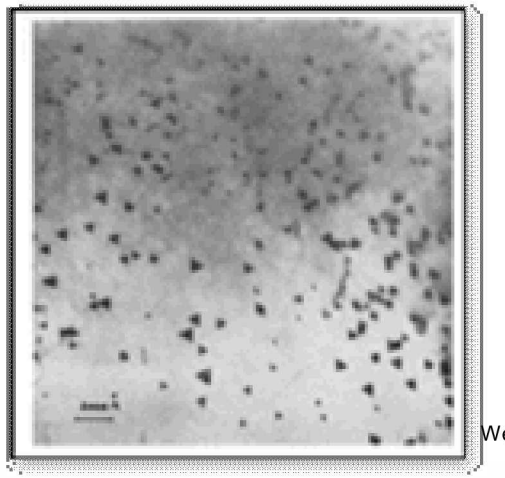


Bubbles



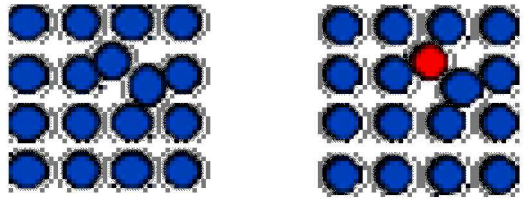
Han et al. (2012)

Stacking Fault Tetrahedras



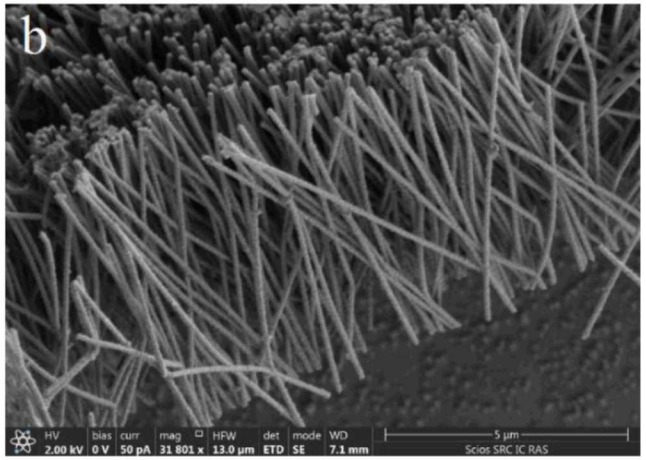
Wesdorp et al. (1964)

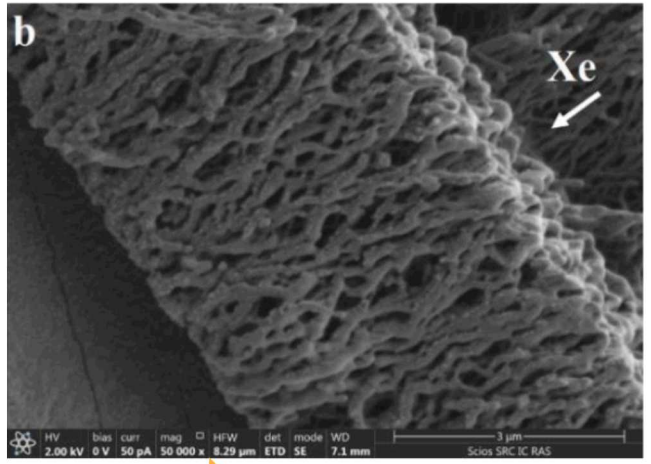
Interstitials



Radiation Damage Accumulation in Nanowires

Placeholder, will be an animation of damage accumulation in a nano-rod, file was to big with the animation in place.



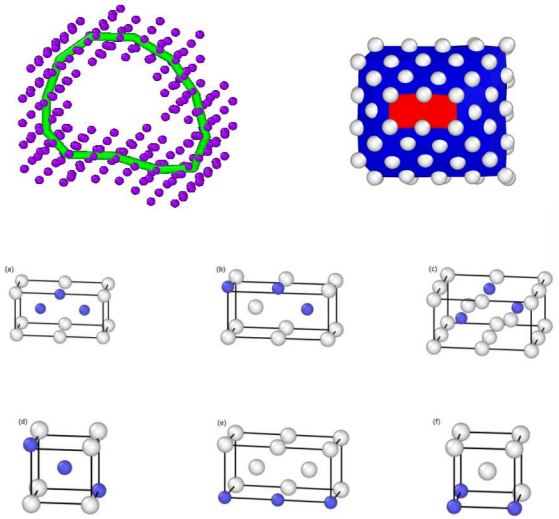


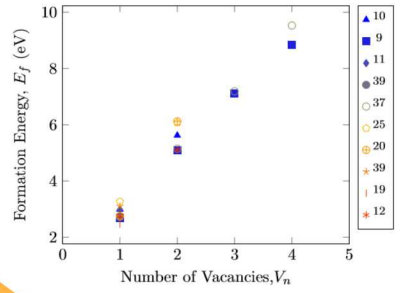
Adapted from Bedin et al. (2017)

Irradiation by Xe^+ Ions

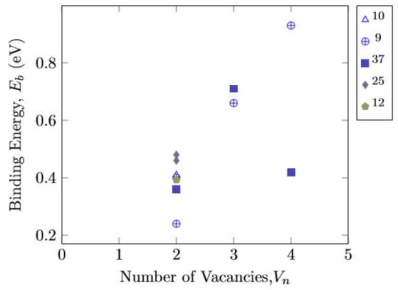
Accumulation of defects due to heavy ion bombardment

Bridging the gap between atomistic and meso-scale simulations

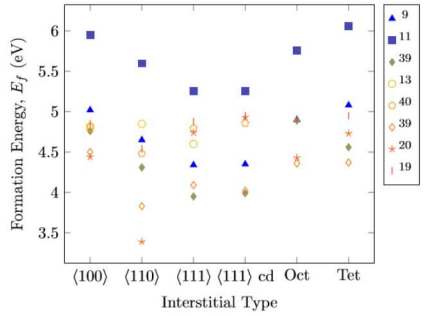




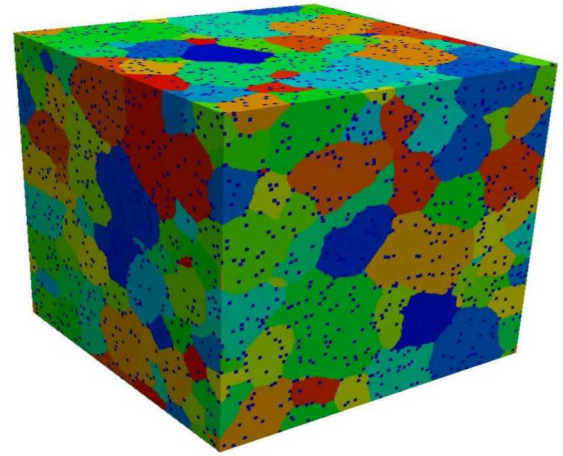
(a)Vacancy formation energy, E_f



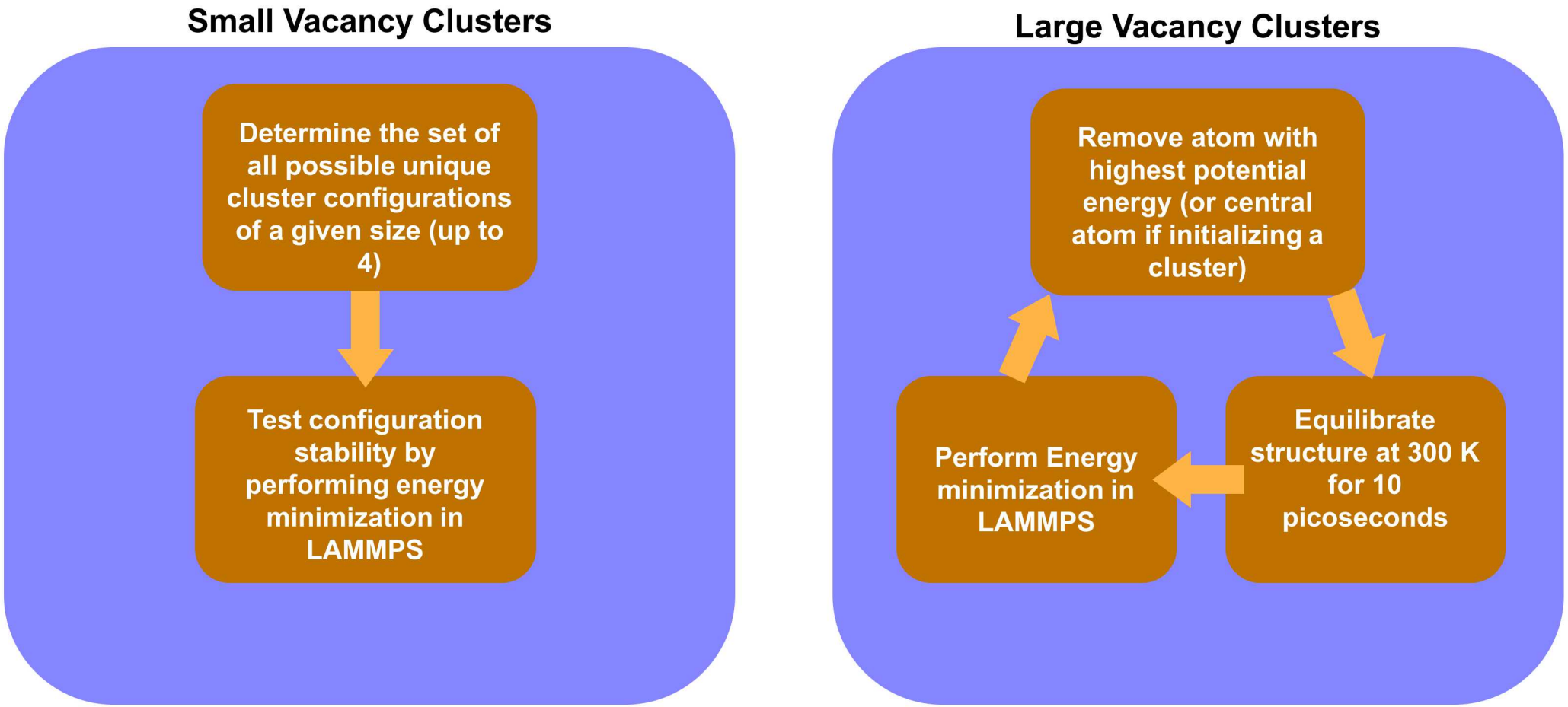
(b)Vacancy binding energy, E_b



(c)SIA Formation Energy, E_f

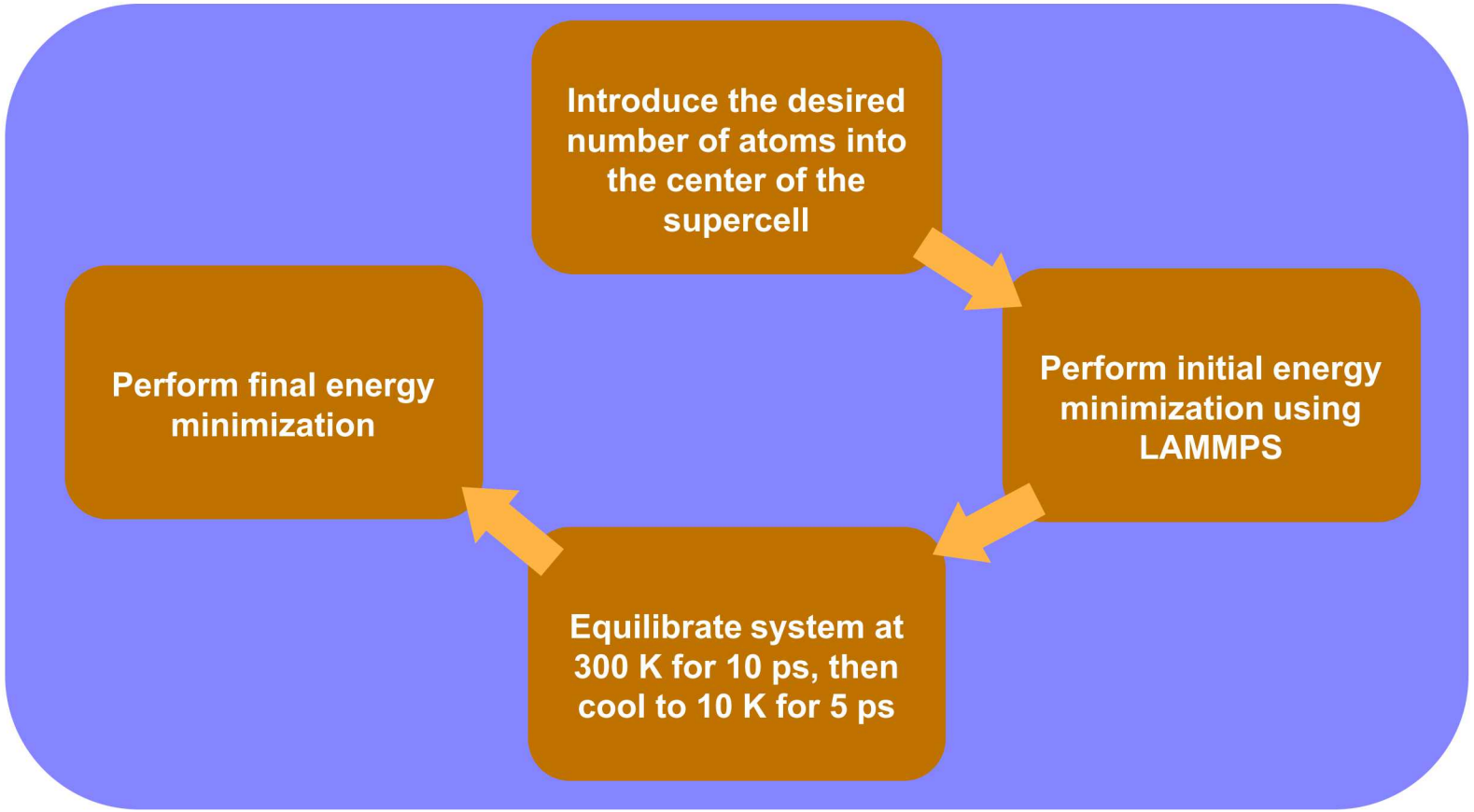


Methods of Defect Cluster Generation



Methods of Defect Cluster Generation

Self-Interstitial Atom Clusters



Calculation of Defect Energetics

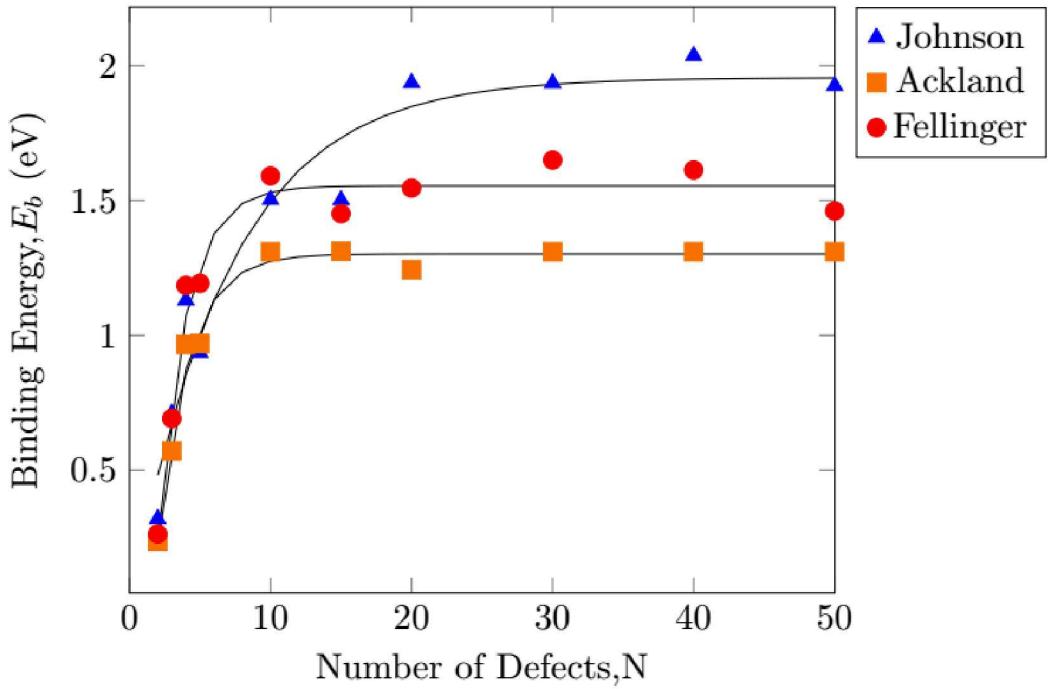
- Formation Energies

$$E_f = E_{N \pm n} - \frac{N \pm n}{N} E_N$$

- Binding Energies

$$E_b = \sum_{i=1}^{K} E_i - E_f$$

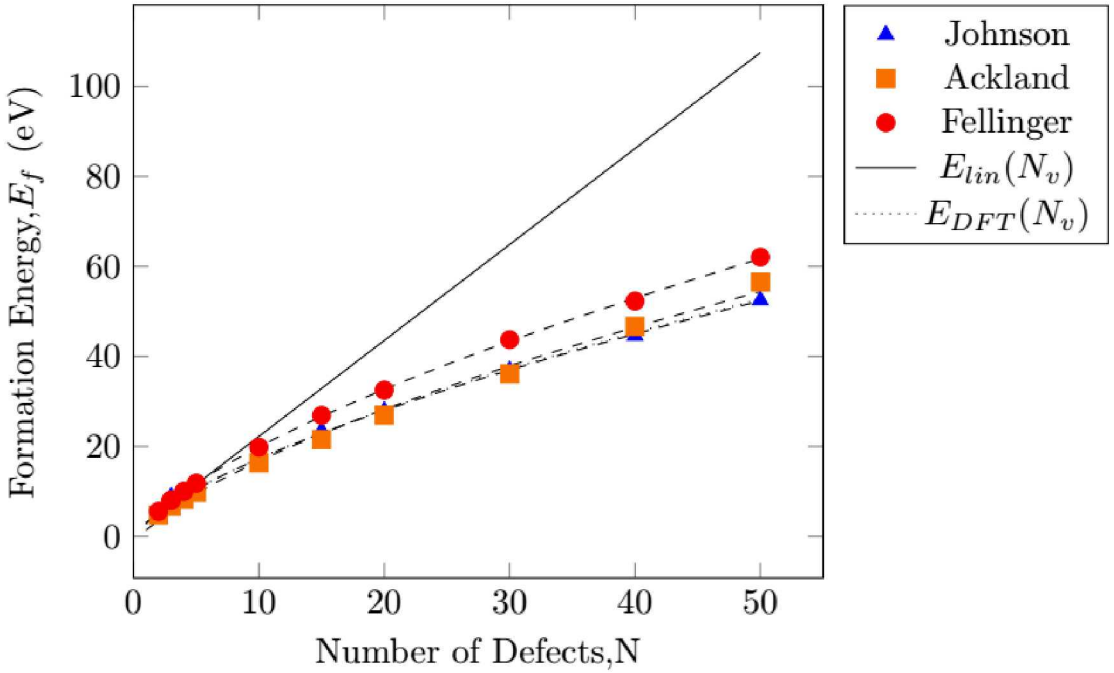
Vacancy Cluster Binding Energy



$$E_b(N_v) = -a_0 exp(-a_1 N_v) + a_2$$

Binding approaches a constant value as cluster size increases

Vacancy Cluster Formation Energy

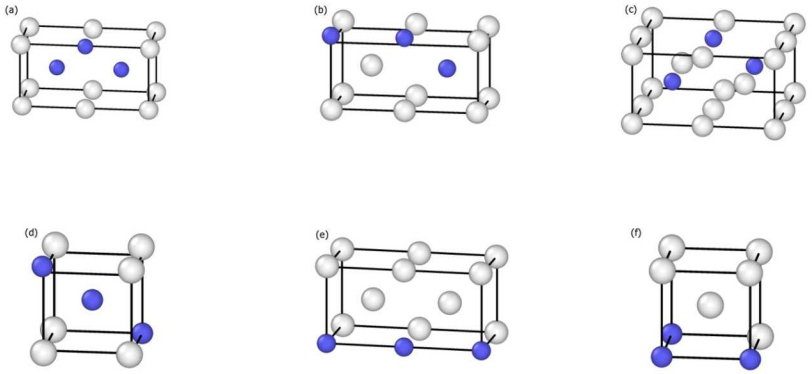


$$E_f(N_v) = a_0 N_v^{\frac{2}{3}} + a_1$$

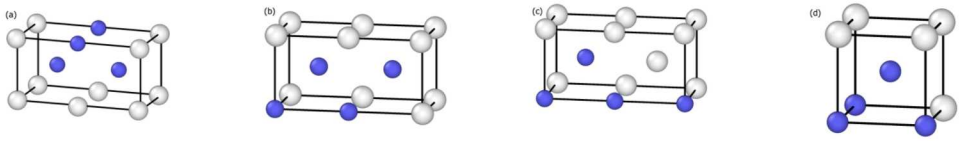
The $N^{2/3}$ term converts the volume of the cluster to the surface area

Vacancy Cluster Configurations

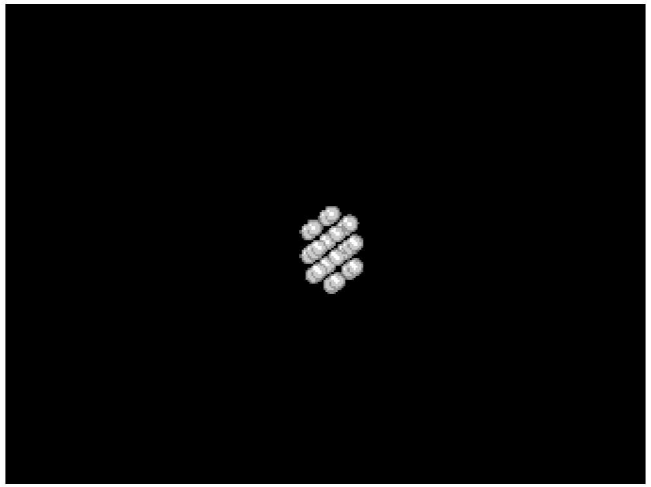
Trivacancies



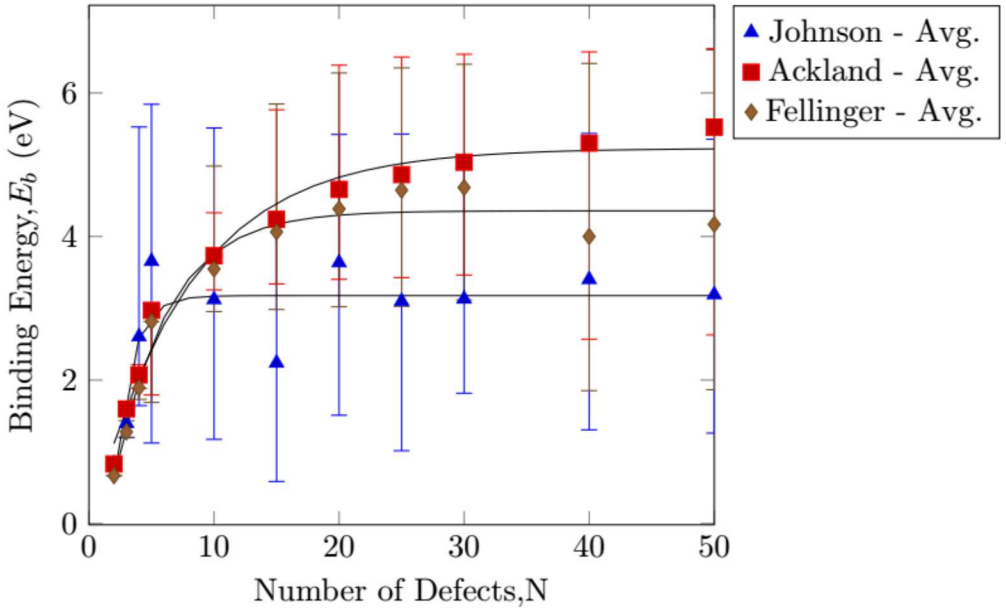
Tetravacancies



Vacancy Clusters



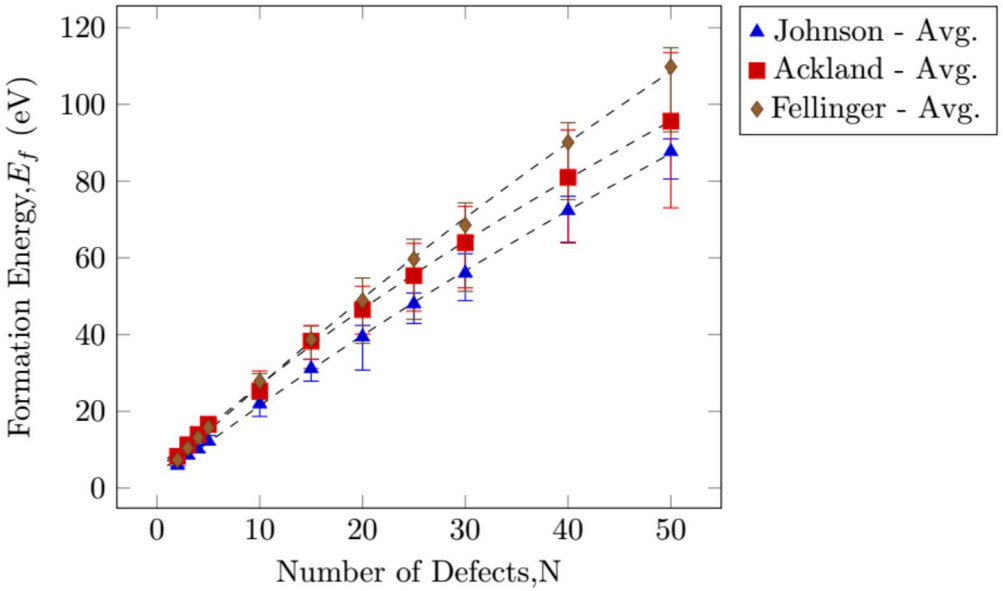
SIA Cluster Binding Energy



$$E_b(N_{SIA}) = -a_0 exp(-a_1 N_{SIA}) + a_2$$

Binding approaches a constant value as cluster size increases

SIA Cluster Formation Energy



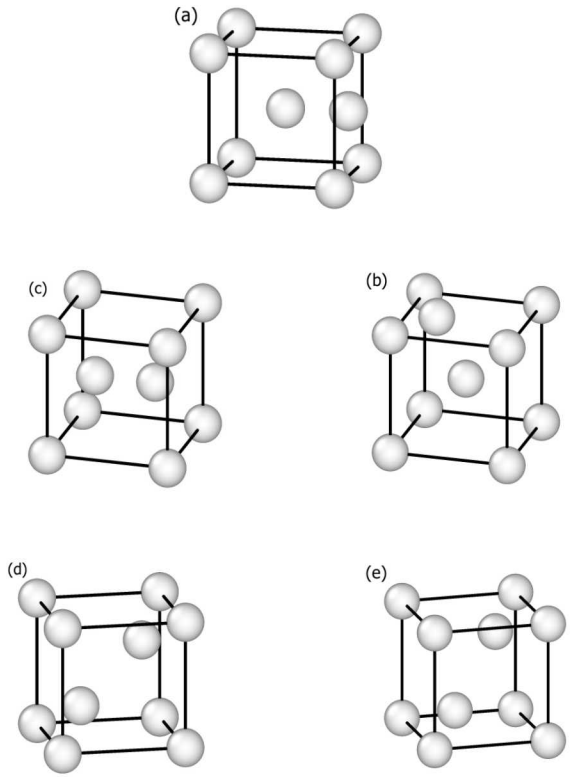
$$E_f(N_{SIA}) = a_0\sqrt{N_{SIA}}ln(N_{SIA}) + a_1\sqrt{N_{SIA}} + a_2$$

This term is an elastic energy term

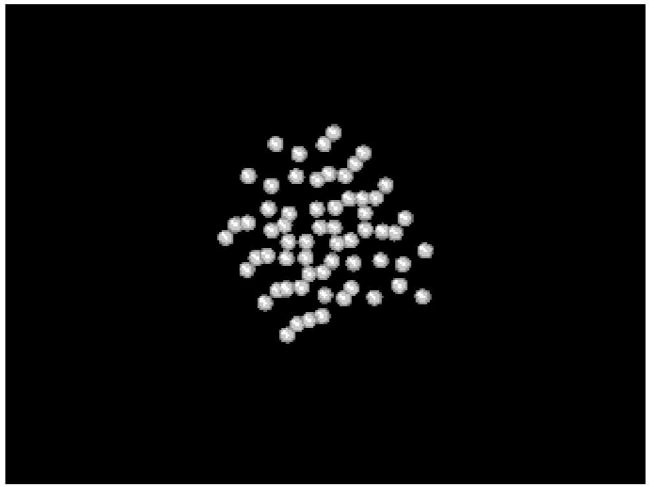
This term is a surface energy term

SIA Cluster Configurations

Single SIA configurations

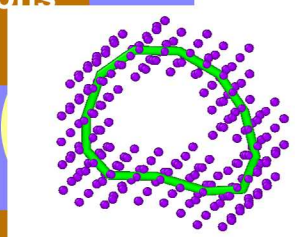


SIA clusters containing 5 to 50 SIAs

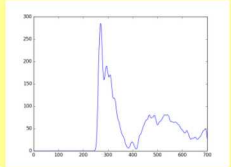


Statistical Characterization of SIA Cluster Geometry

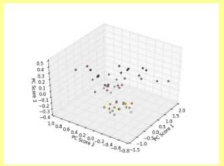
Generate random SIA cluster configurations



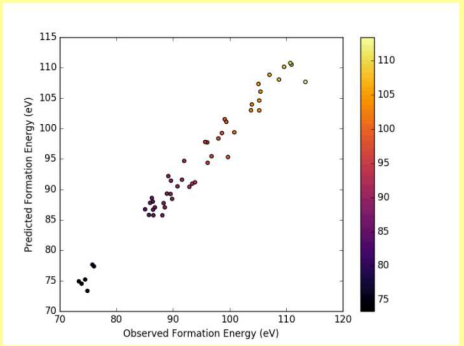
Characterize defect structure by taking the radial distribution function (RDF).



Perform primary component analysis (PCA).



Build linear regression model using PC scores and formation energies



Conclusions

- Formation and binding energies of vacancy and SIA clusters have been predicted for sizes up to 50 vacancies or SIAs using three interatomic potentials.
- Functional forms have been fit to the average formation and binding energies of defect clusters as a function of the number of individual defects.
- Linear regression models can be trained can be trained on and predict the formation energies of SIA clusters containing a set number of SIAs.

Questions