SAND2019-5370C

Exceptional service in the national interest

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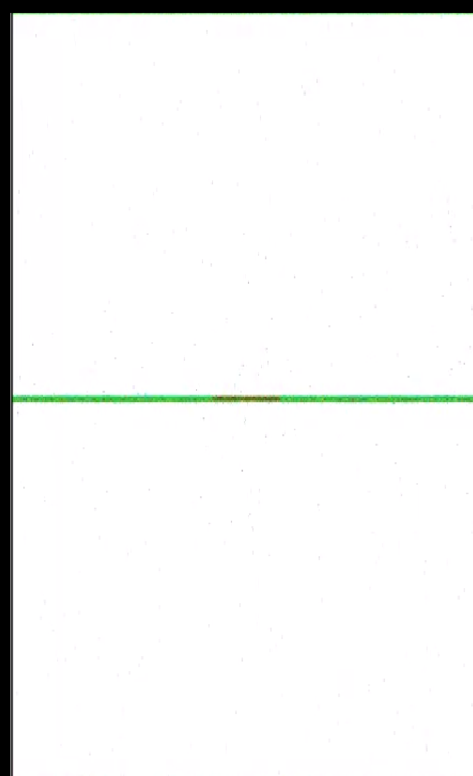
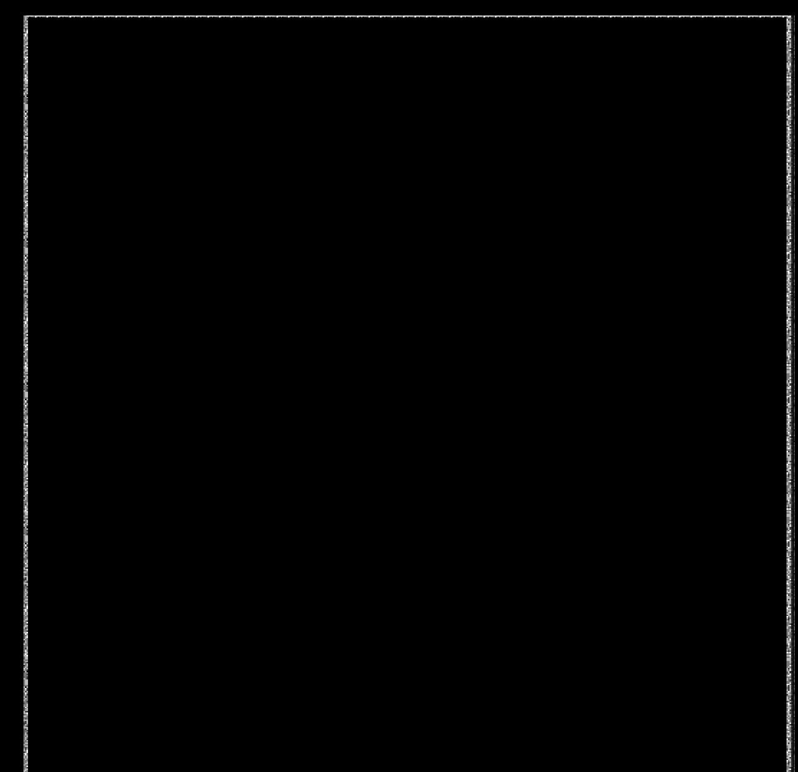
INFLUENCE OF STRUCTURE AND CHEMISTRY ON THE RADIATION RESISTANCE OF BOUNDARIES





RÉMI DINGREVILLE
CENTER FOR INTEGRATED NANOTECHNOLOGIES (CINT)
SANDIA NATIONAL LABORATORIES

SAND2019-XXXX PE

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Multidisciplinary & Collaborative Research

Sandia National Laboratories

- **Graduate students**

  W. Barrow* (M.S., U. Arkansas), **A.Y. Dunn* (Ph.D., GaTech)**, **E. Chen (Ph.D., GaTech)**, **D. Vizoso (Ph.D., GaTech)**, D. Aksoy (Ph.D., U. Florida), P. Zarnas (Ph.D., Northwestern U.)

- **Postdocs**

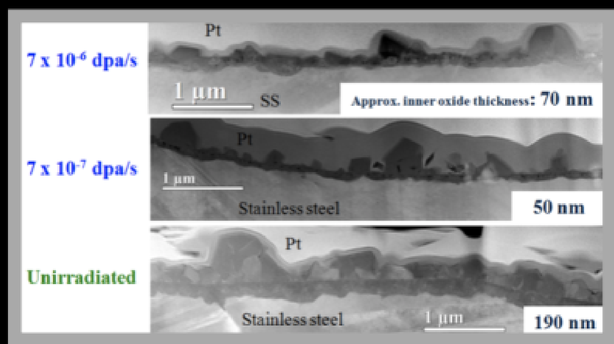
  C.J. O'Brien (now staff), **P.A. Juan (now at Kairos)**, J. Stewart, C. Kunka

- **External Collaborators**

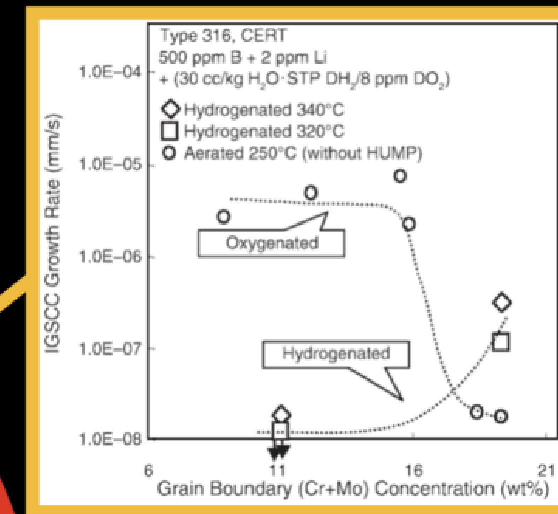
  O. Anderoglu (UNM), T.J. Balk (U. Kentucky), S. Berbenni (CNRS, France), L. Capolungo (LANL), **C. Deo (GaTech)**, E. Kim (UNLV), C. Harrington (EPRI), C. Hin (VaTech), J. Qu (Tufts U.), D. Rudland (NRC), A. Schleife (UIUC), **P. Singh (GaTech)**, D.E. Spearot (U. Florida), R.A. Regueiro (CU Boulder)

Materials Aging & Degradation in Extreme Environments

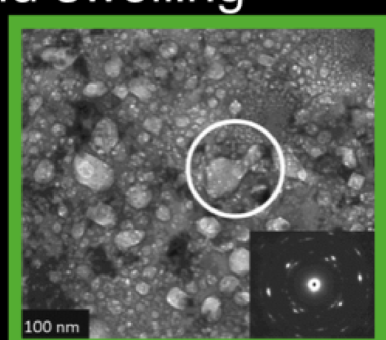
Irradiation-assisted corrosion

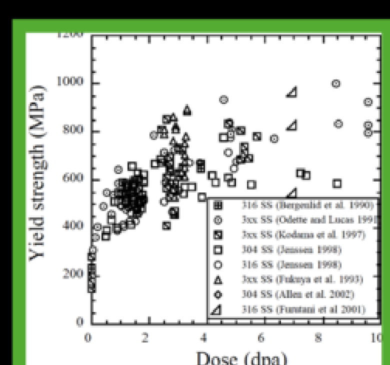


Stress Corrosion Cracking



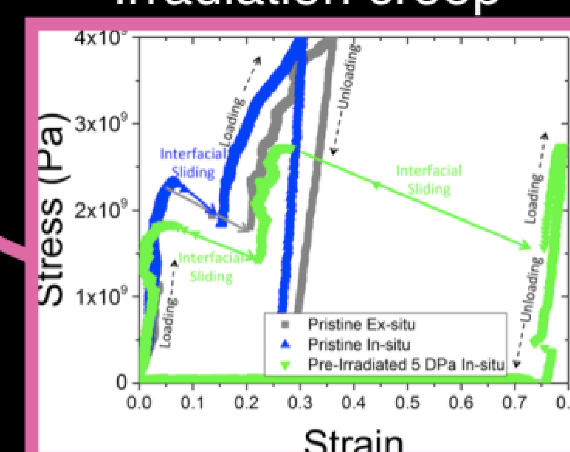
Void swelling





Hardening

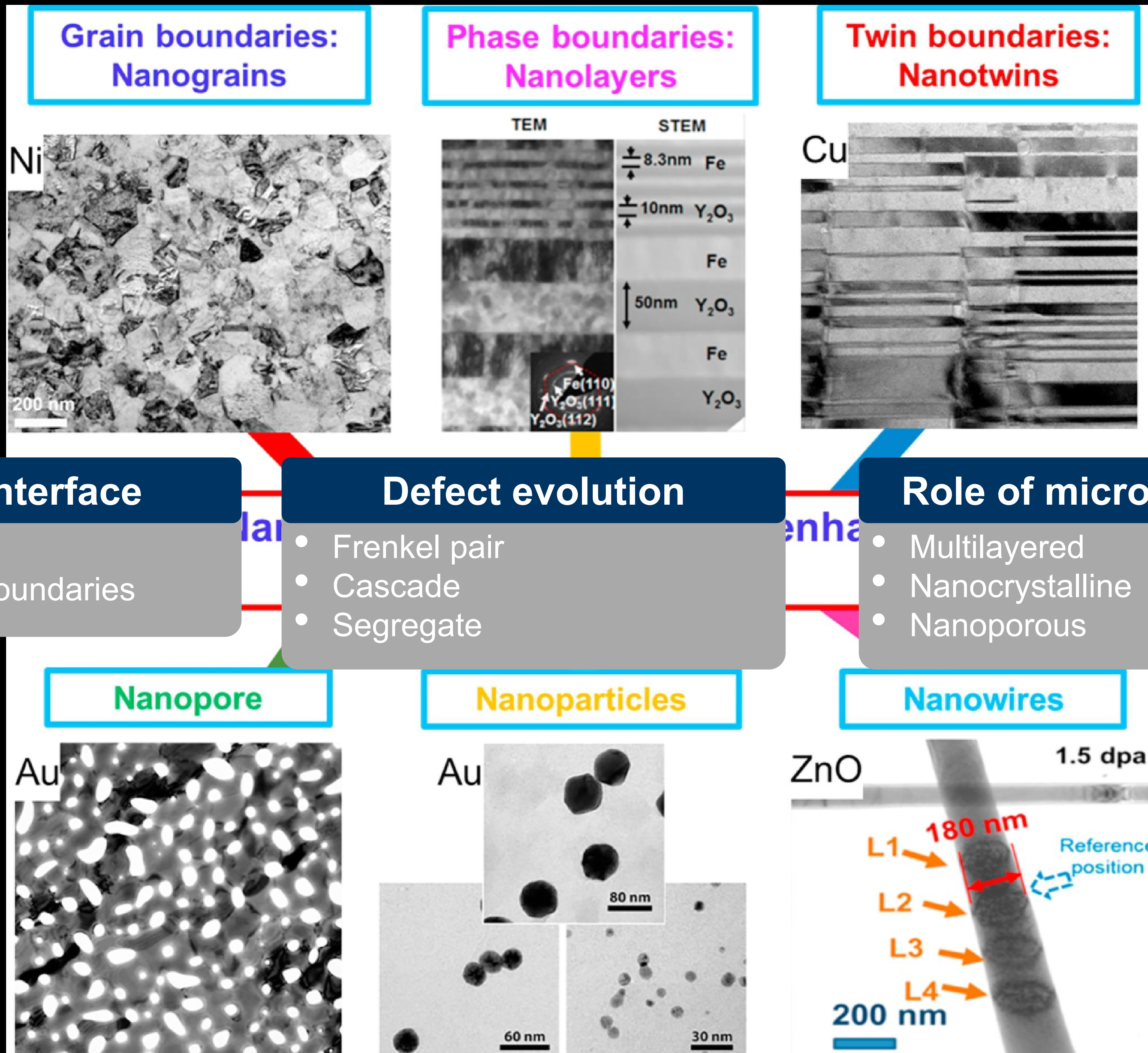
Irradiation creep



"The only source of knowledge is experience."

— Albert Einstein (1879-1955) —

NANOSTRUCTURING AS A SOLUTION TO MANAGING DEGRADATION UNDER EXTREMES



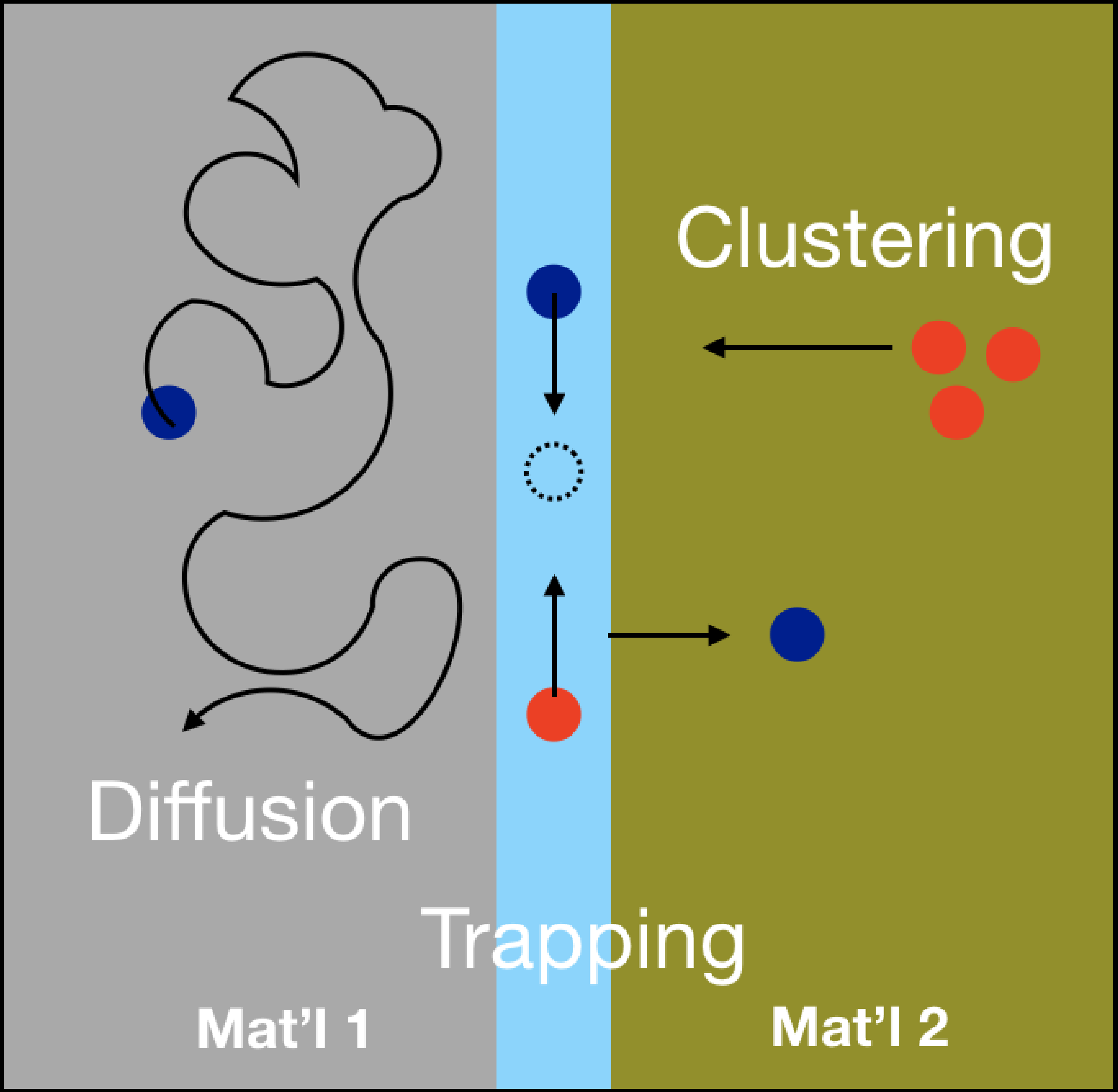
Role of interface
- Free surface,
- Grain/phase boundaries

Defect evolution
- Frenkel pair
- Cascade
- Segregate

Role of microstructure
- Multilayered
- Nanocrystalline
- Nanoporous

ang et al. (2018) *Prog. Mater. Sci.*]

What Makes an Interface a "Good" Interface?

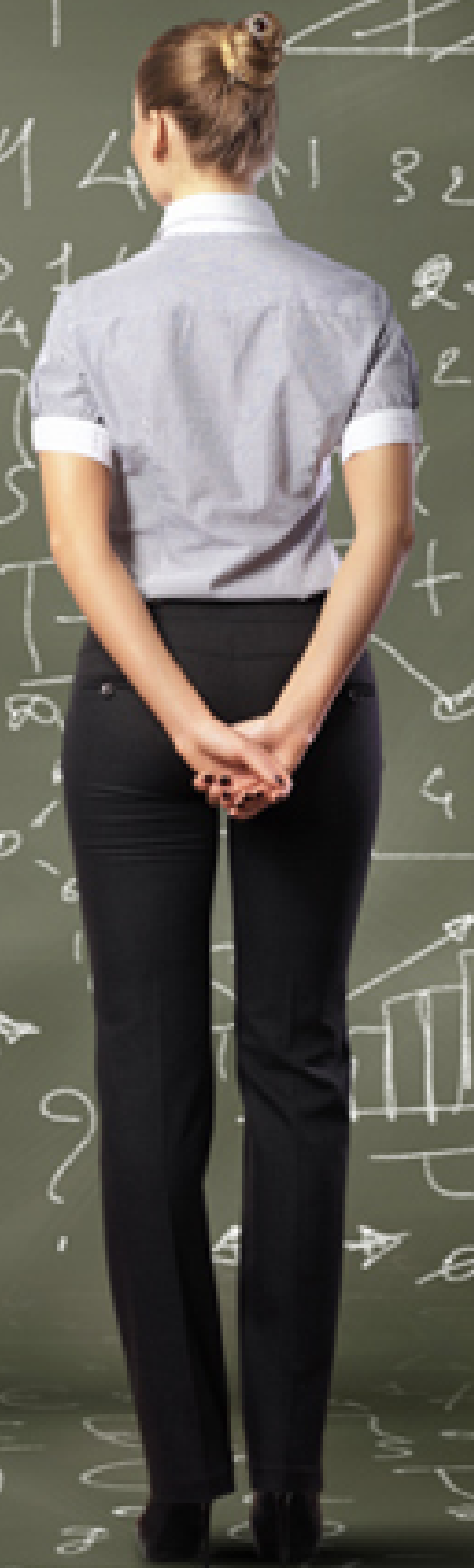


Excess volume
Low formation of defects at interface
Defect core delocalization at interface

Accelerate code qualification of new materials

Beyond "just" theory & simulation:

- **Broad range of interfaces**
  - Limited when using atomistic models
- **Interface as imperfect sinks**
  - Limited when using mesoscale models
- **Beyond model (interfacial) systems**
  - Limited with most models

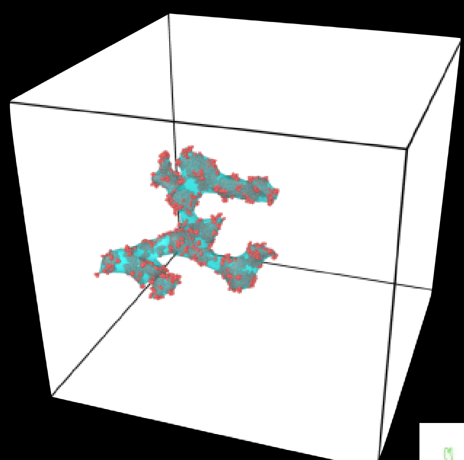


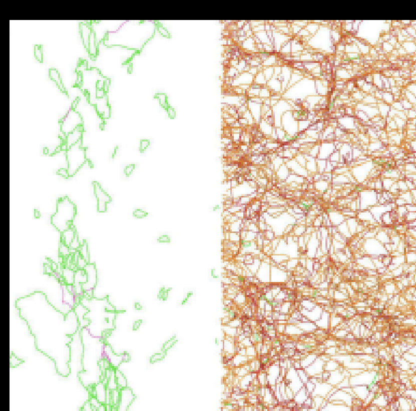
Mature Modeling Techniques at Relevant Scales

Å nm μm cm

ps ns μs s

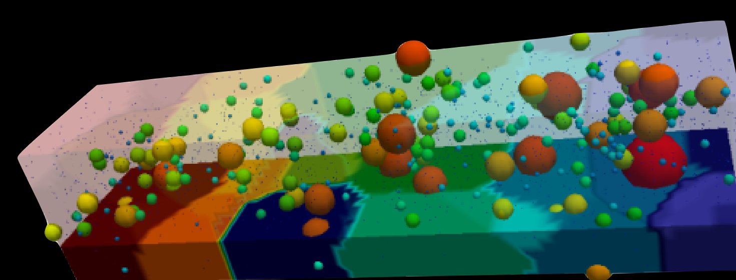
Defect scale

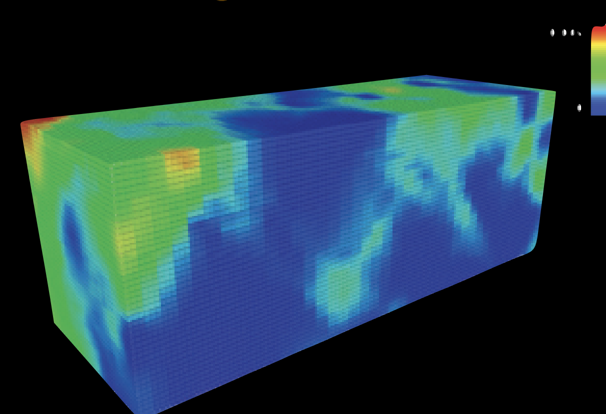




Defect production

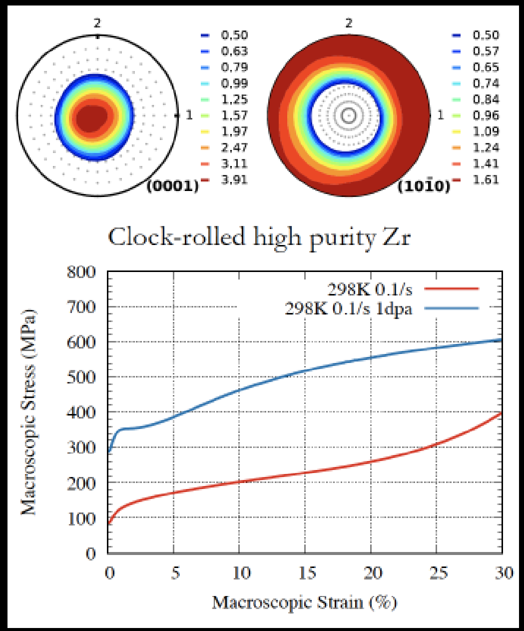
Grain scale





Defect evolution

Structure scale



Defect effects

Model Damage Production at the Atomic Scale Using Molecular Dynamics: Ballistic Effects

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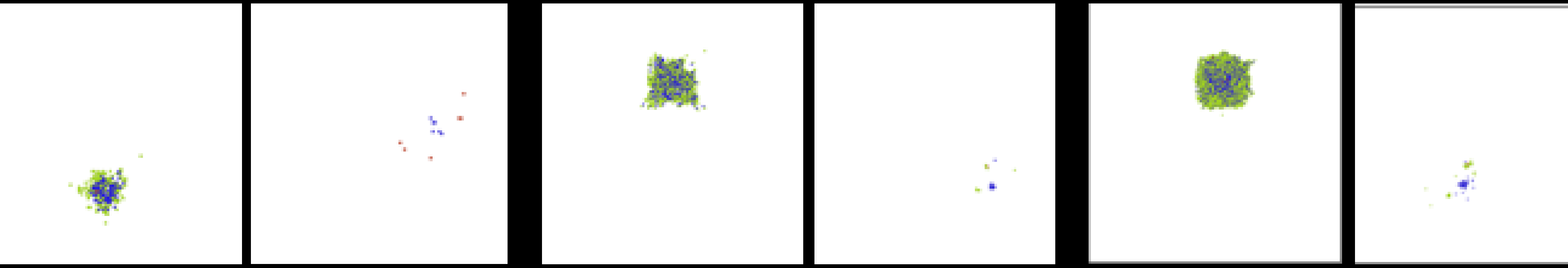
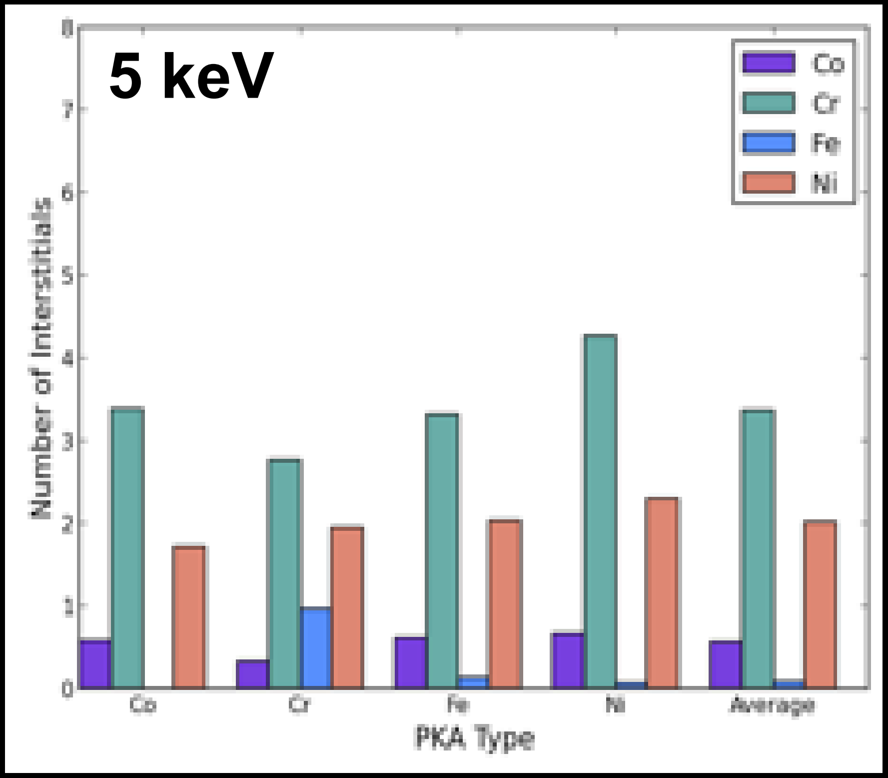
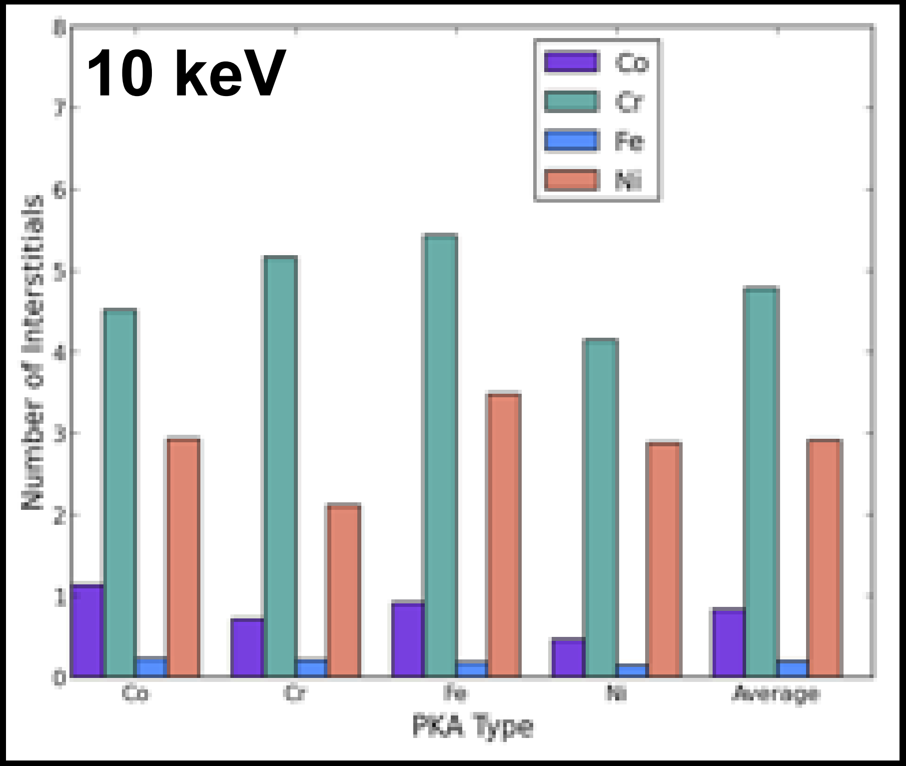
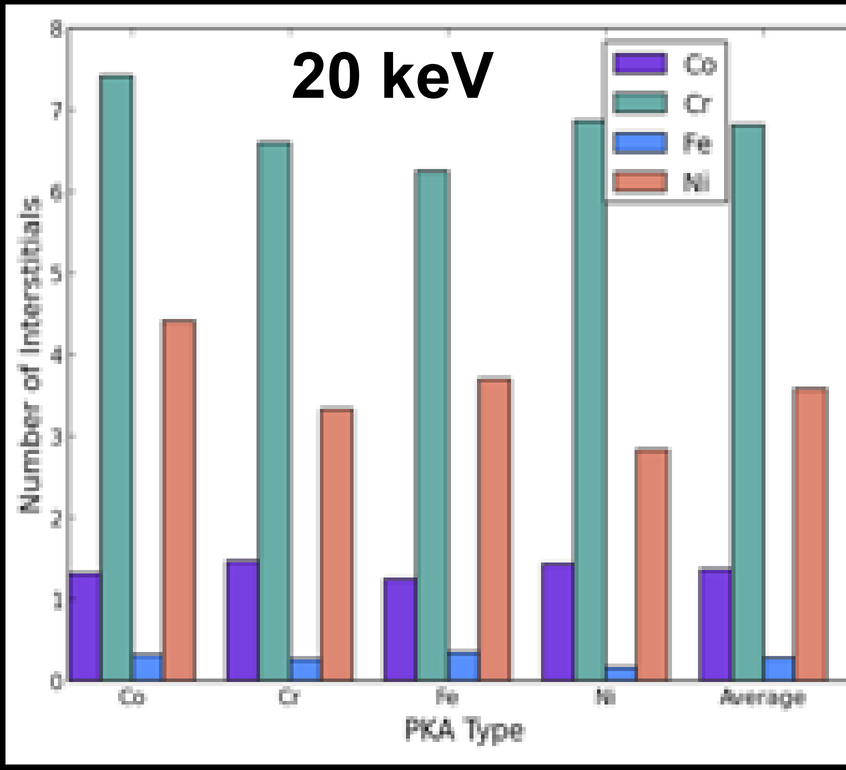
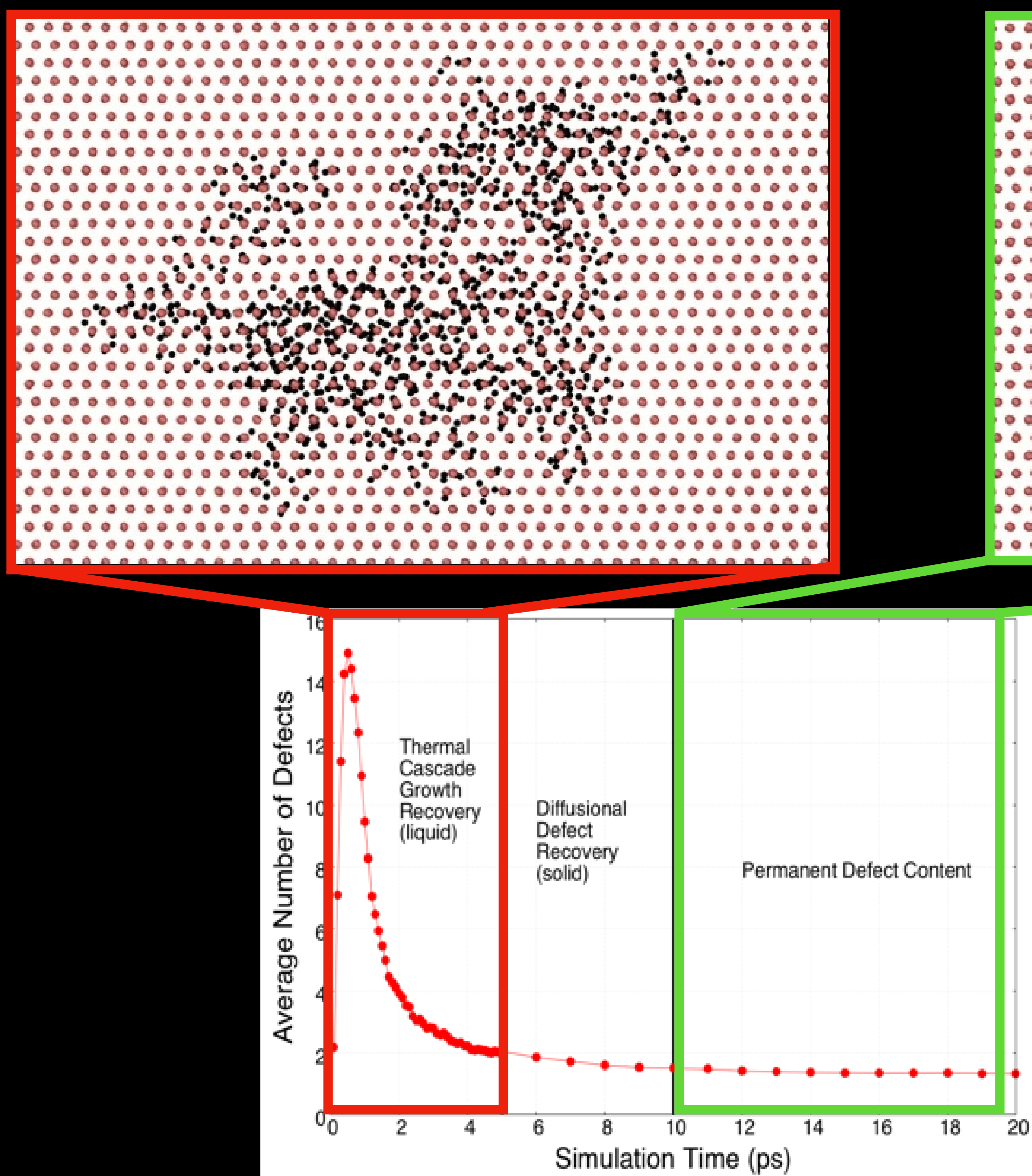


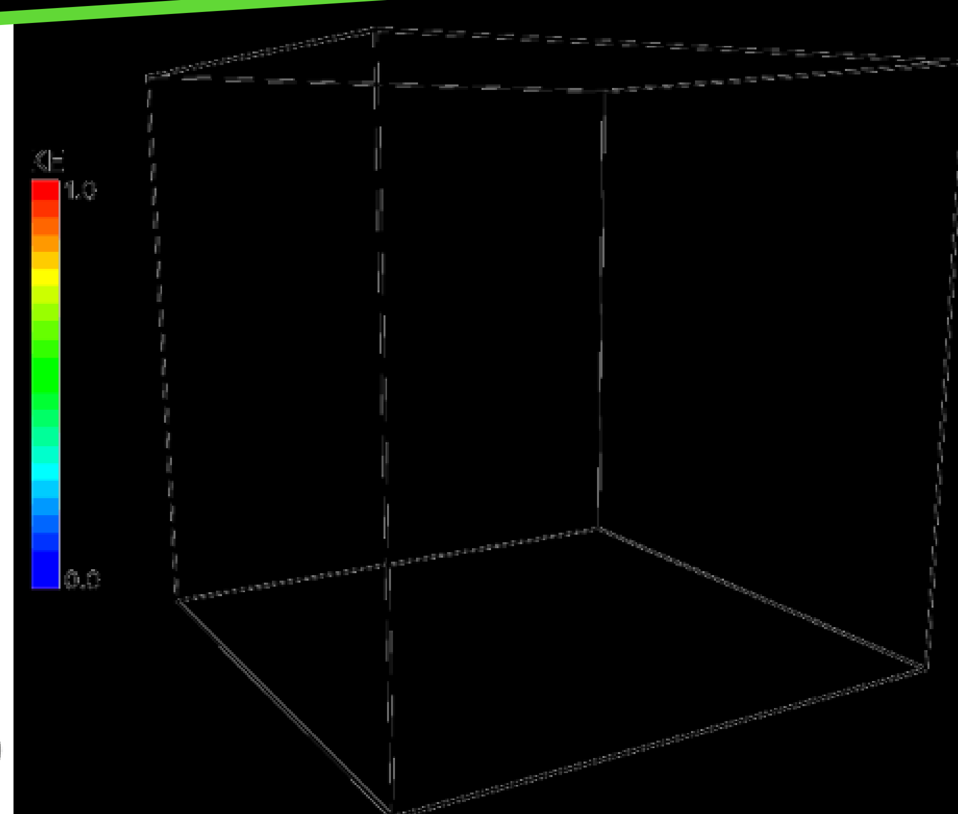






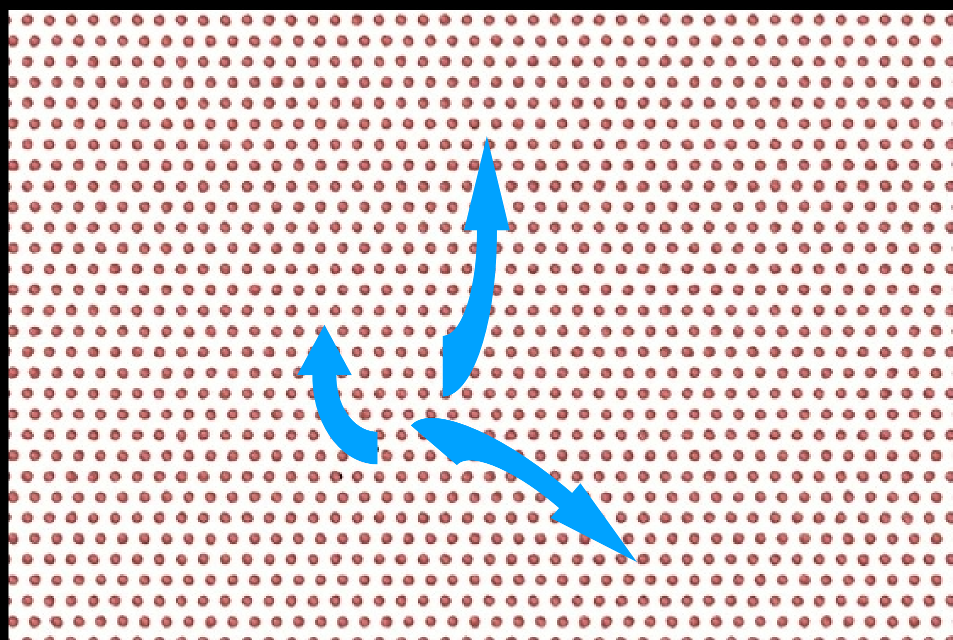
Model Damage Production at the Atomic Scale Using Molecular Dynamics: Ballistic Effects



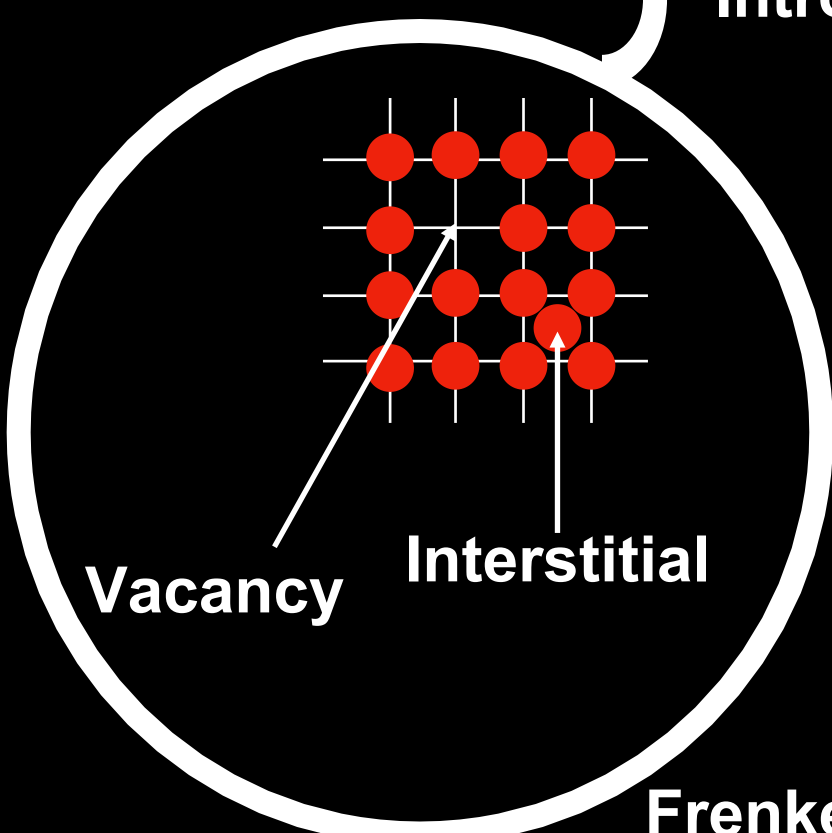


Model Damage Production at the Atomic Scale Using Molecular Dynamics: Dose Effects

Recombination regime:



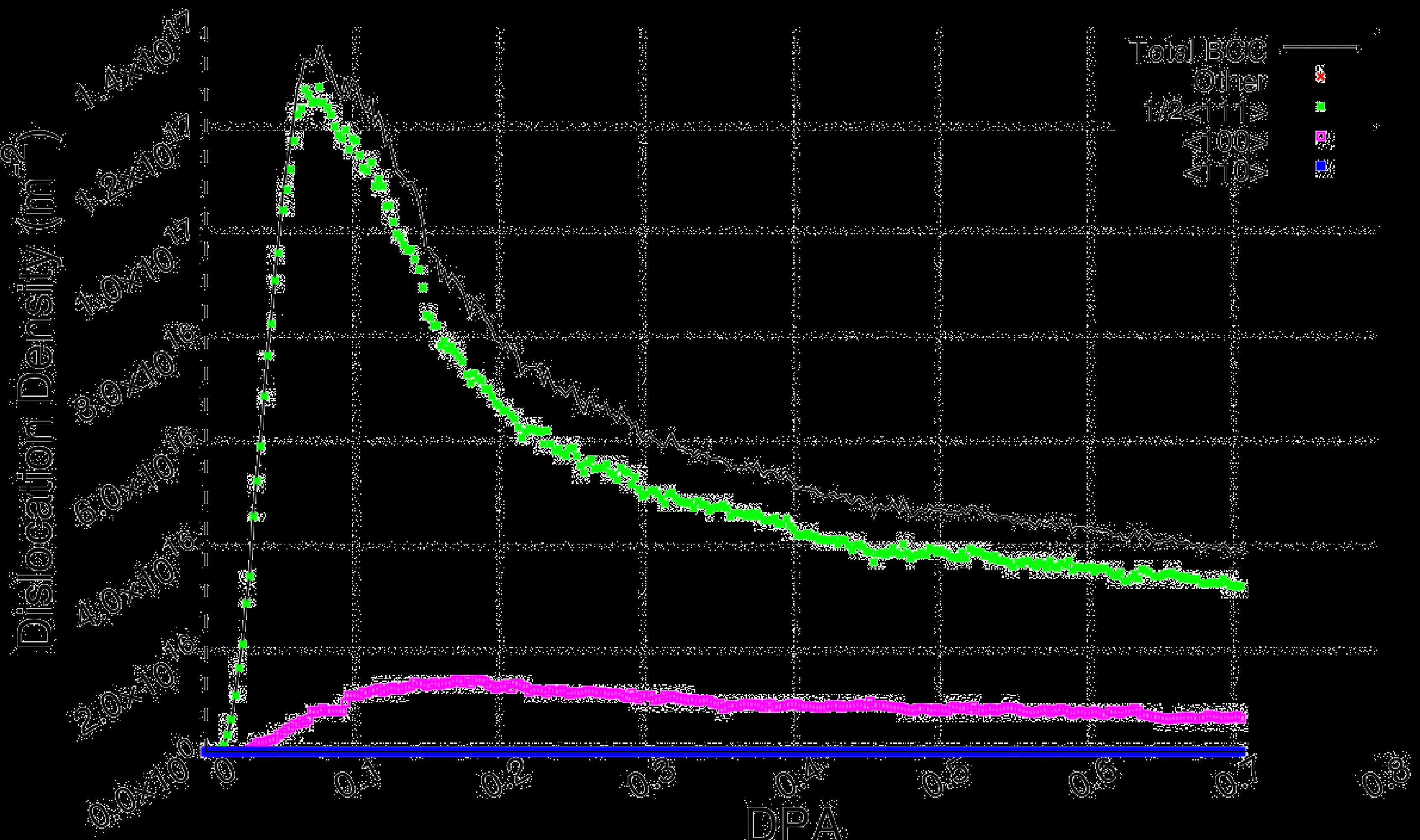
Introduction N FPs every 2ps



Frenkel pair

- Maximum allowed displacement (SRIM)
  - First collision range
- Effective dose rate: 8×10^{-4} dpa/ps
- 300 K, constant P, T

Defect Accumulation Mechanisms



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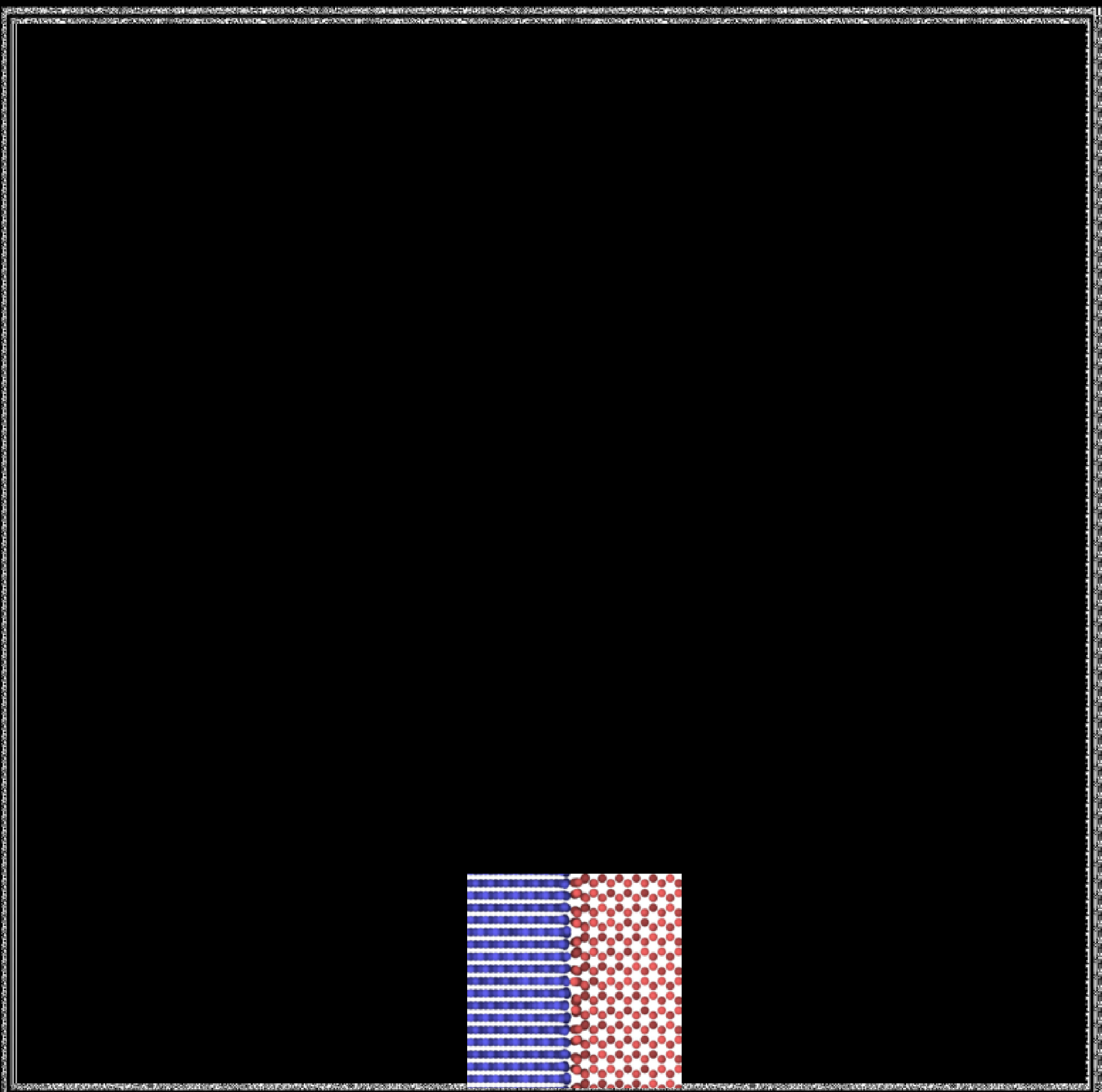
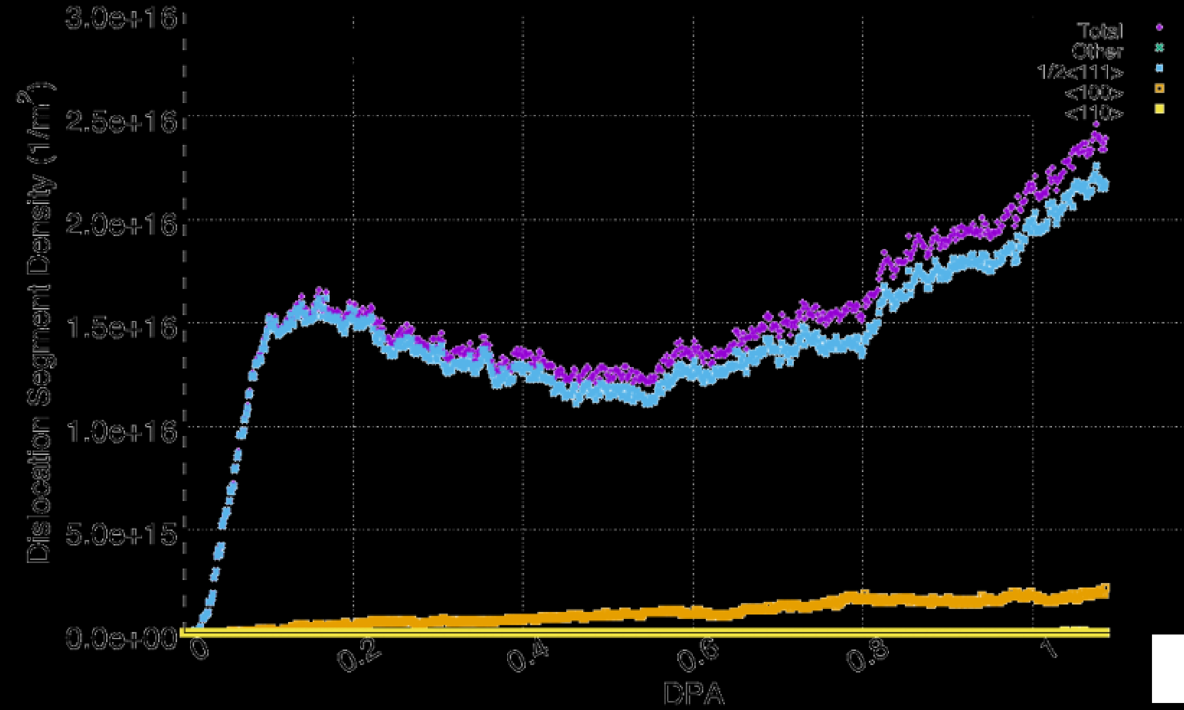
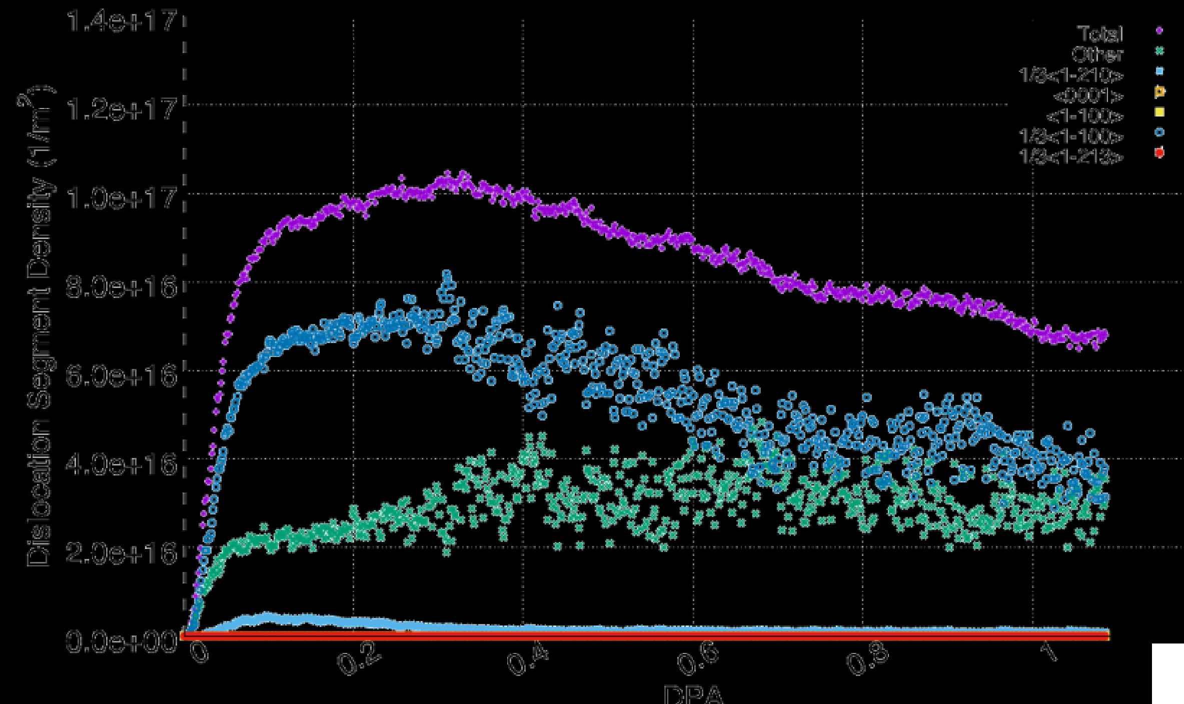
Understanding Radiation Resistance of Phase Boundaries Through Atomistic Modeling







Collaboration with E. Chen and C. Deo (GaTech)

[Chen et al. (2019) *J. Mater. Res.*]

Understanding Interfacial Embrittlement Through Atomistic Modeling

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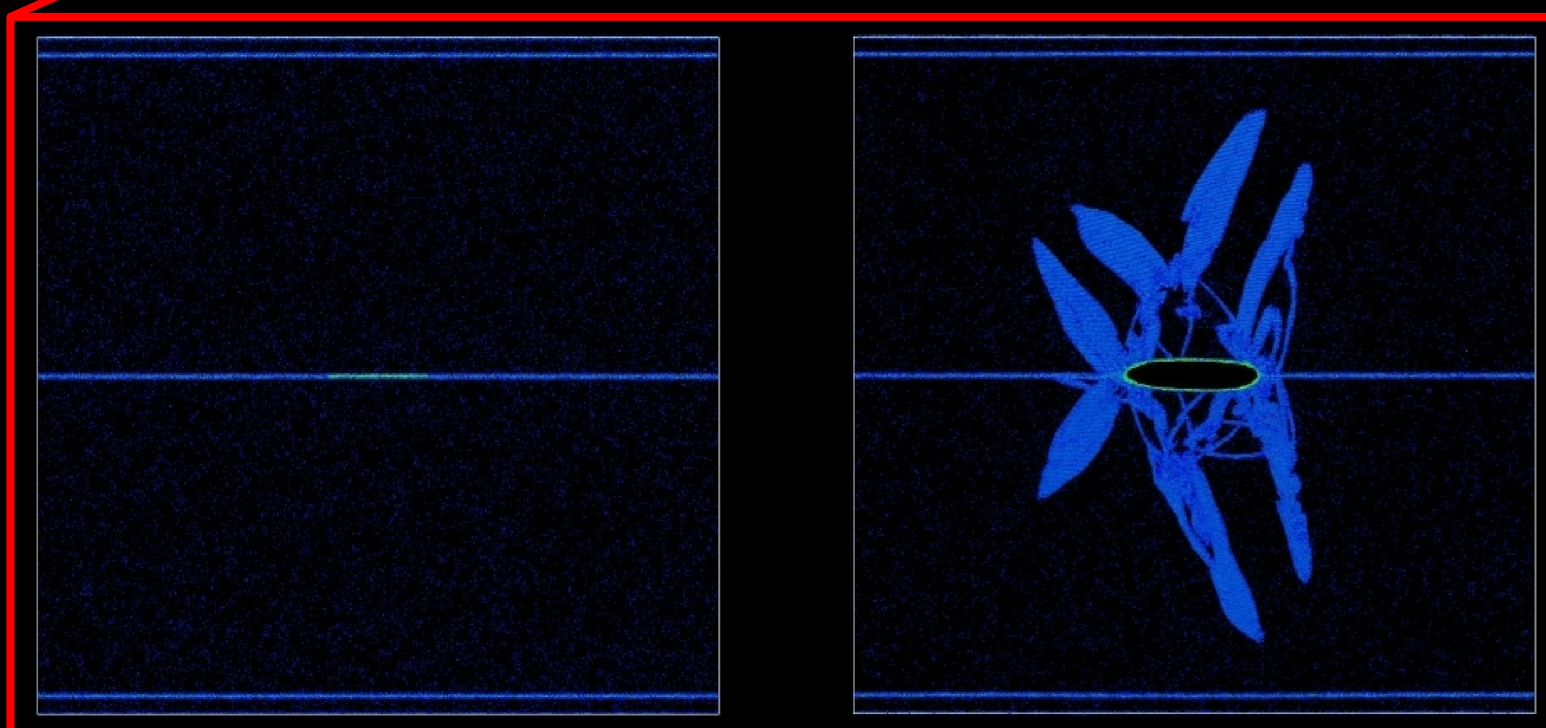
Step 1
Build grain boundary structure

Step 2
Equilibrate system under pre-tension

Step 3
Introduce atomically sharp crack

Step 4
Allow crack growth under pre-tension

Step 5
Averaging to extract decohesion form



- **Avoids having to artificially impose a boundary velocity**

Collaboration with D. Spearot (U Florida)

[Dingreville et al. (2017) *Sci. Rep.*]

UNDERSTANDING INTERFACIAL EMBRITTLEMENT THROUGH ATOMISTIC MODELING

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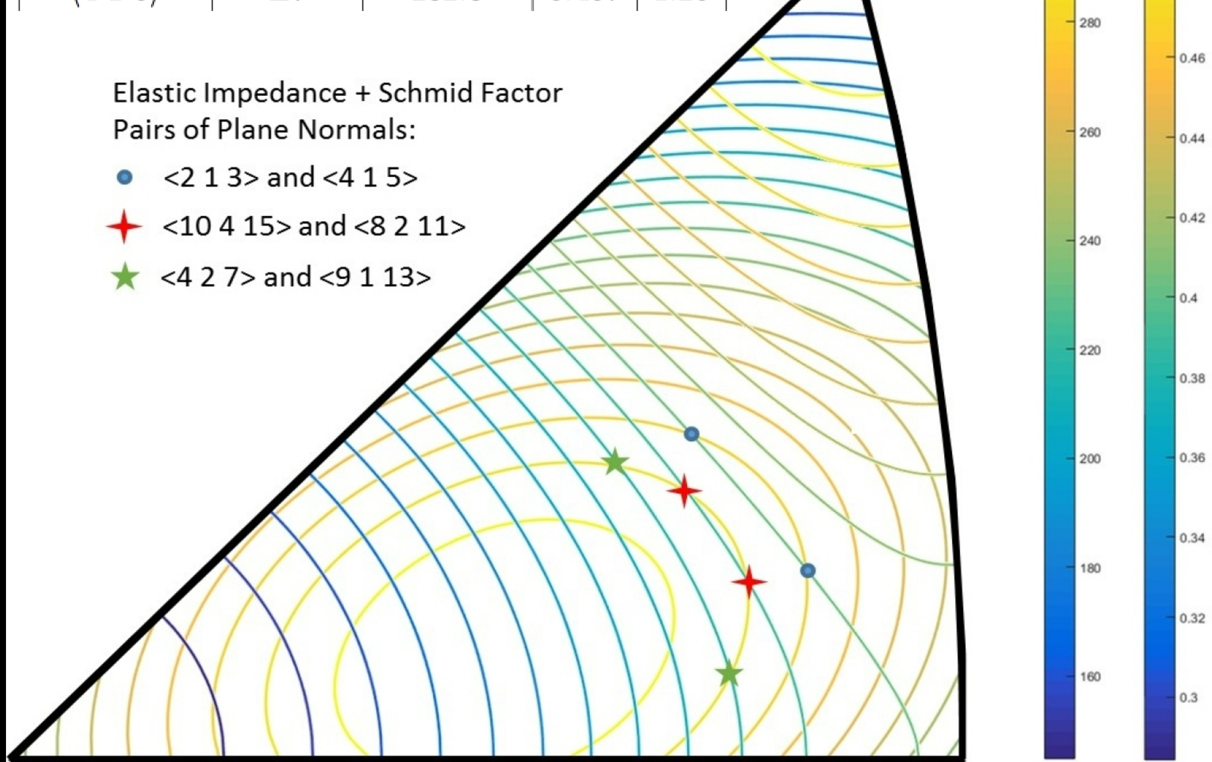
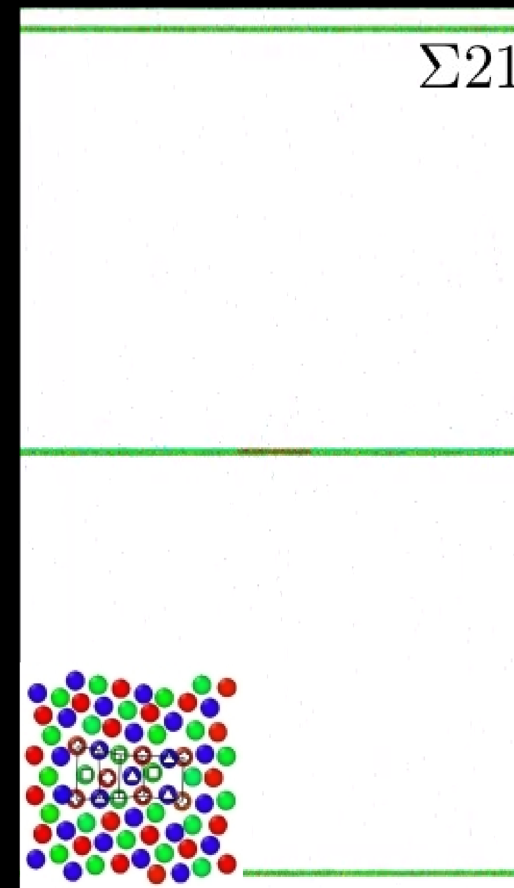
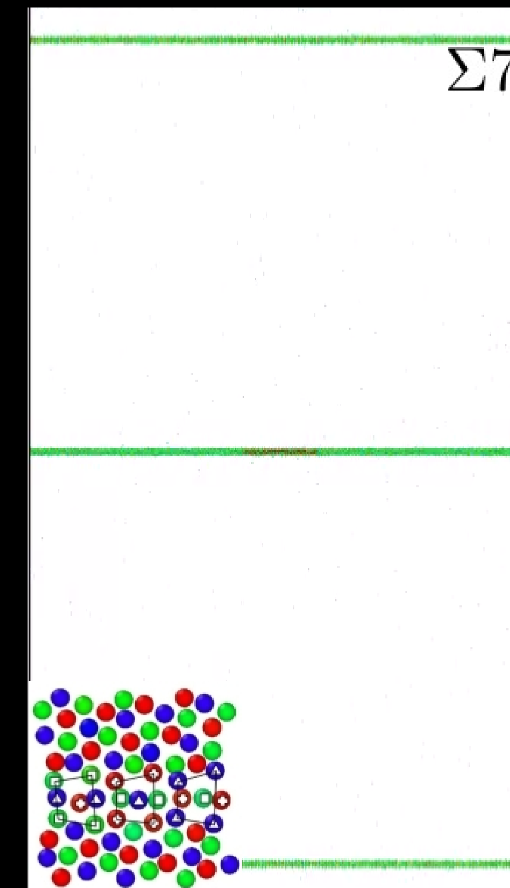
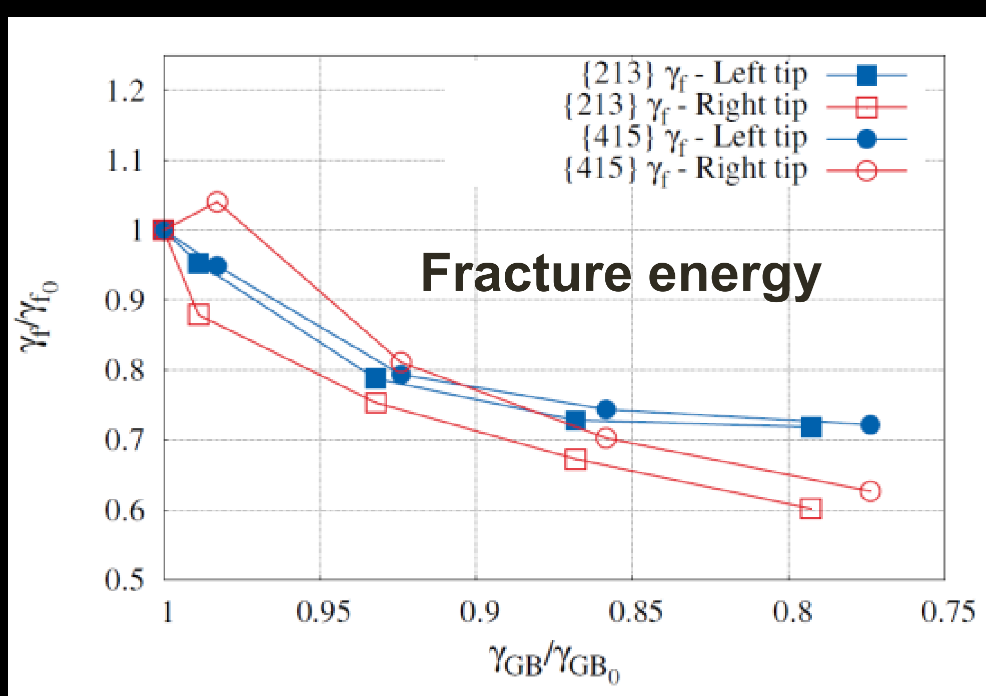
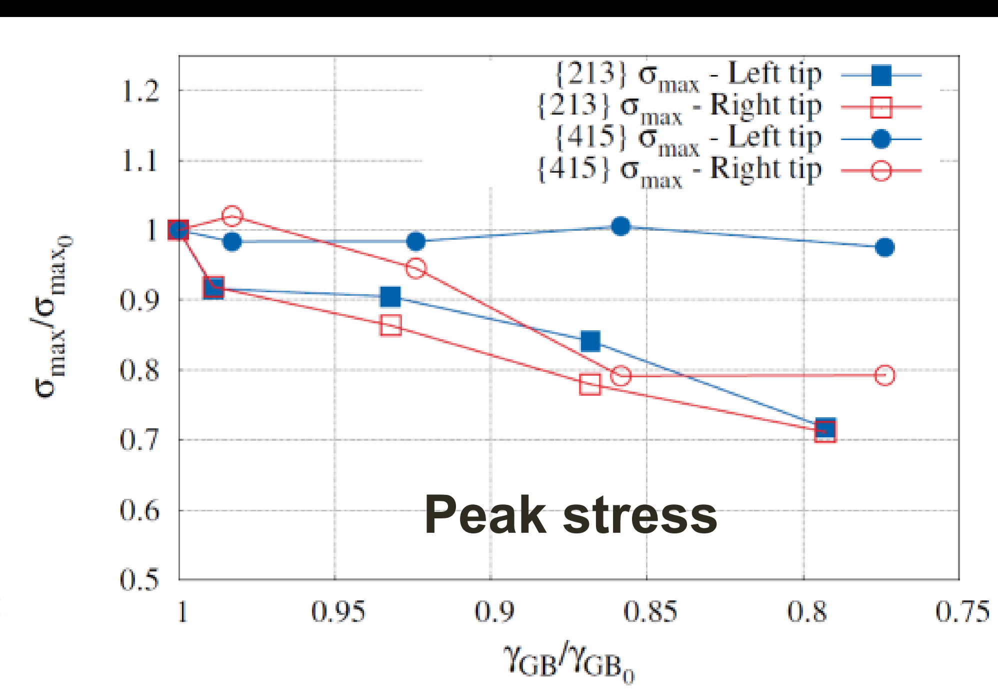
GB Normal	GB CSL	$E_{\vec{X}}$ [GPa]	μ	R_μ
⟨2 1 3⟩	Σ21	232.6	0.467	1.33
⟨4 1 5⟩	Σ7	232.6	0.467	1.20











Collaboration with D. Spearot (U Florida)

[Dingreville et al. (2017) *Sci. Rep.*]

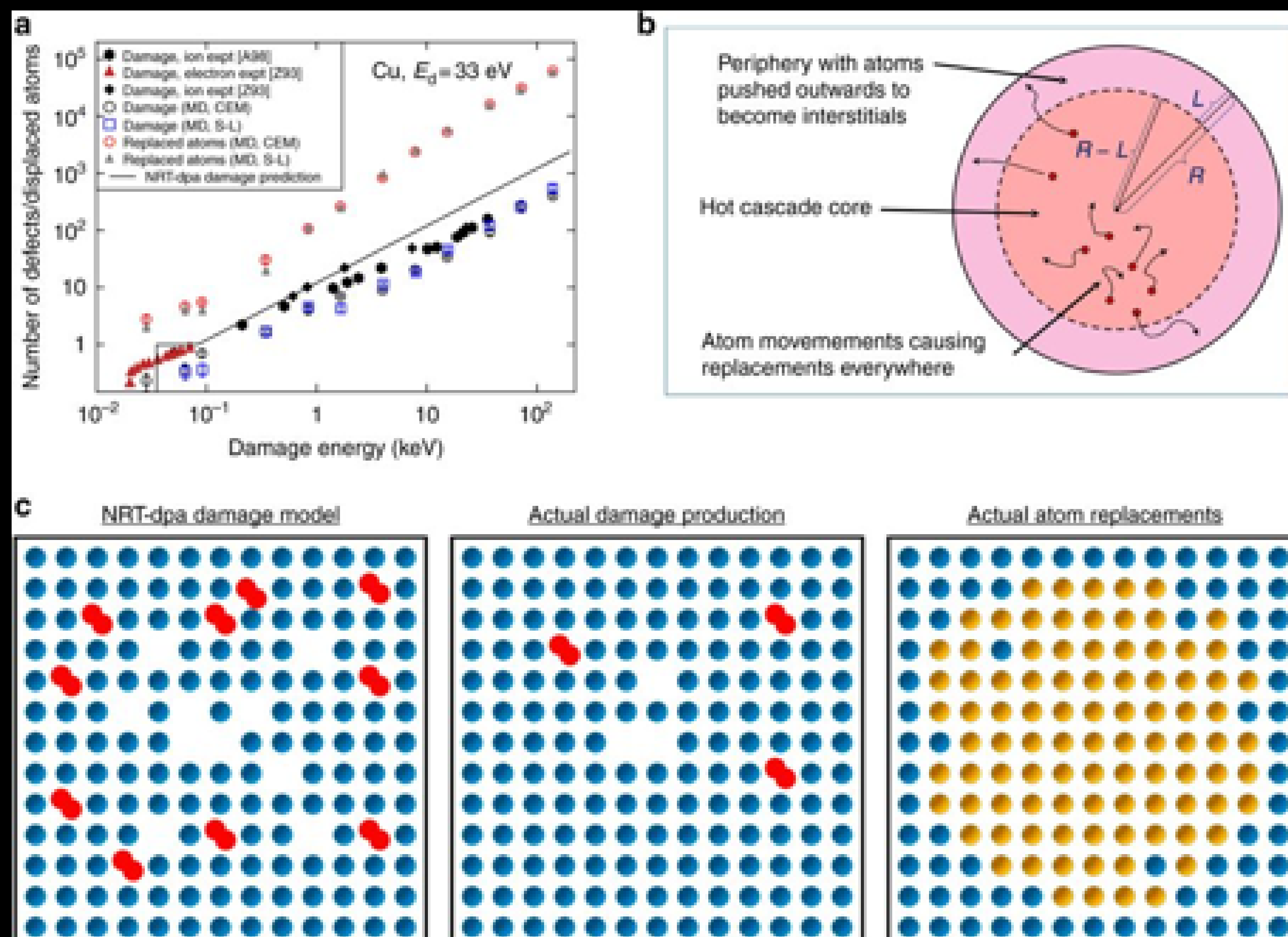
TAKE HOME MESSAGE:

- **Simulations of the accumulation of radiation-induced defects near interfaces**
  - Insights into interplays of defect-defect interactions
  - Role of atomic intermixing
  - Beyond FPA?

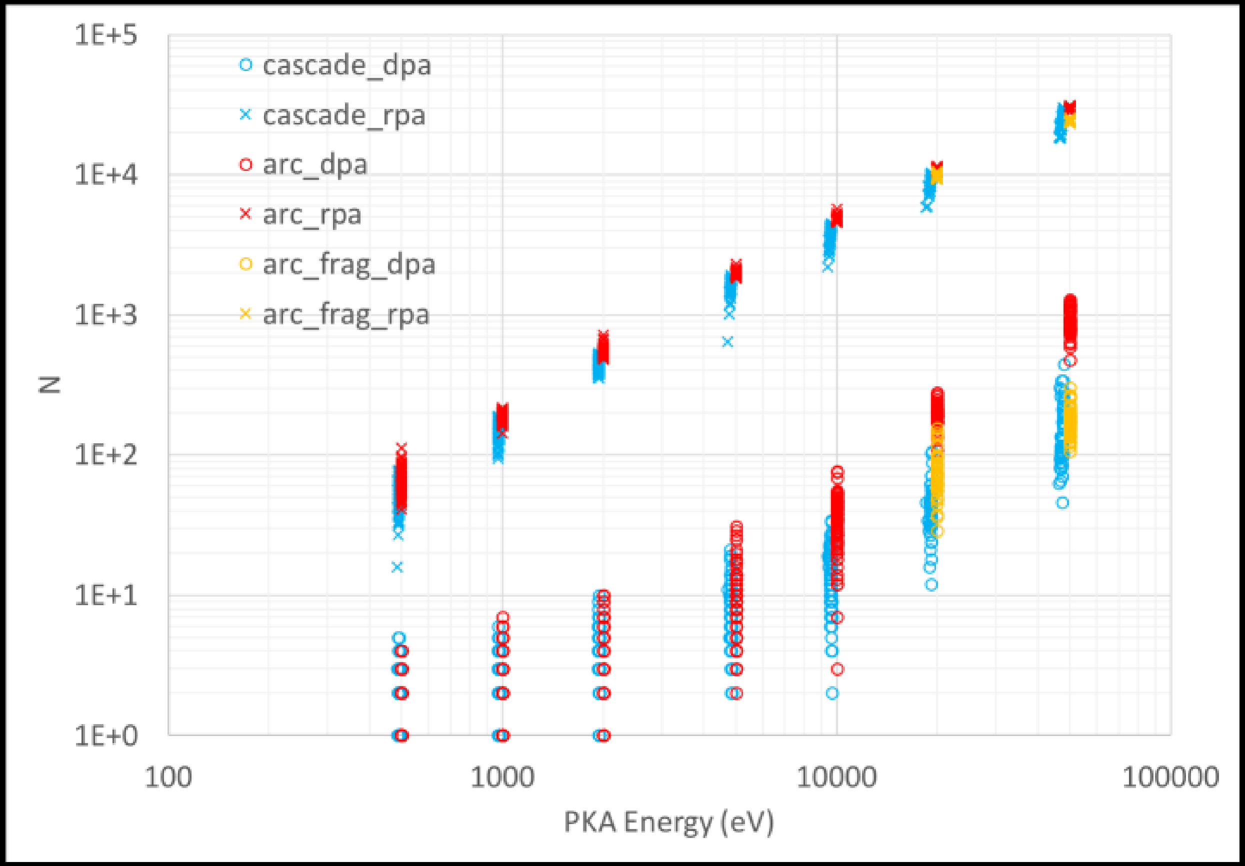
- **Most promising opportunities are at the crossroads of theory & simulation, data analytics, structure & property characterization, chemistry, …**
  - High-throughput simulations for screening
  - Upscaling to materials qualification
  - Integration into regulatory context?

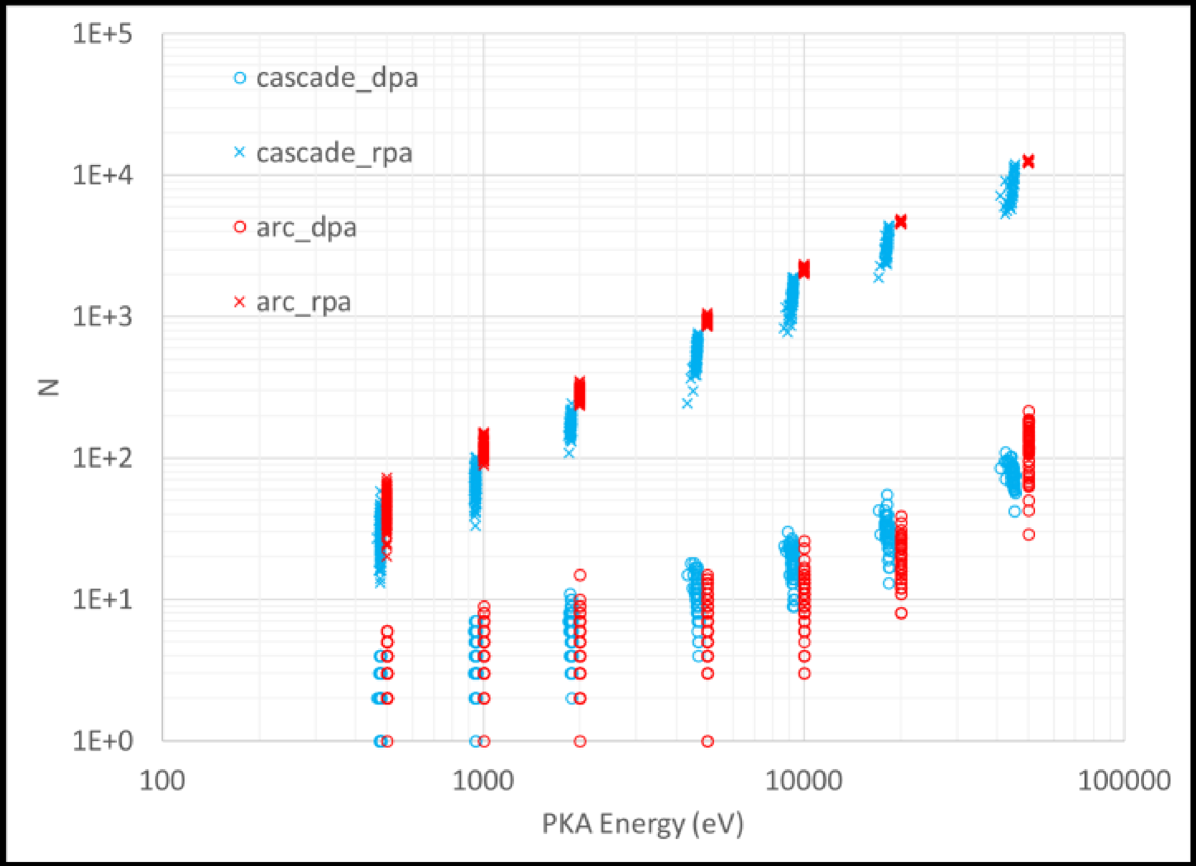
BEYOND FPA

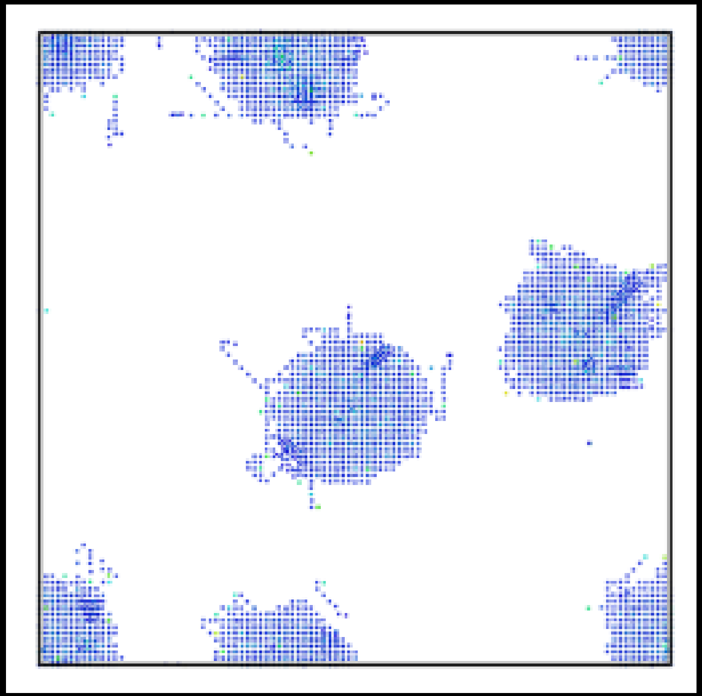
$$N_{\mathrm{dpa/rpa}}\left(T_d\right) = \begin{cases} 0 & \text{for} \quad \mathrm{T_d} < \mathrm{E_d} \\ 1 & \text{for} \quad \mathrm{E_d} < \mathrm{T_d} < \dfrac{2\mathrm{E_d}}{0.8} \\ \dfrac{0.8 T_d}{2 E_d}\xi_{\mathrm{dpa/rpa}} & \text{for} \quad \dfrac{2\mathrm{E_d}}{0.8} < \mathrm{T_d} < \infty \end{cases}$$



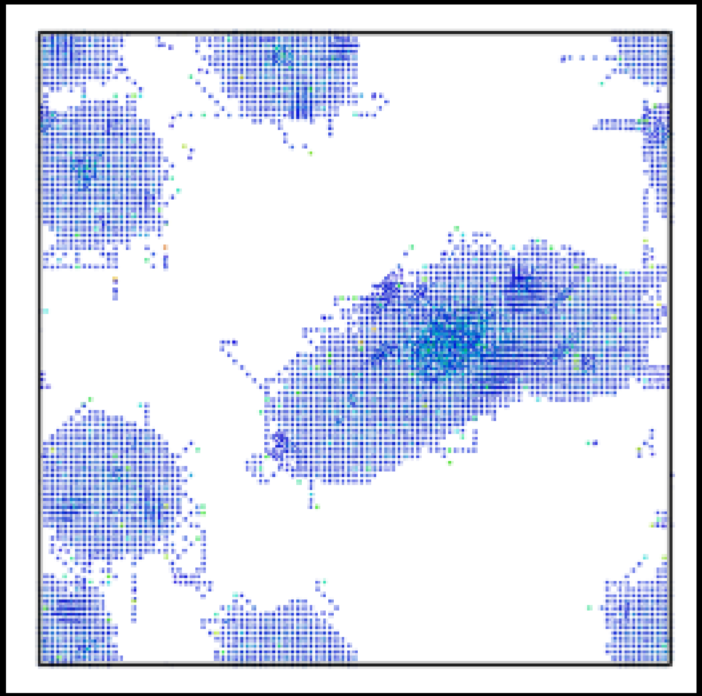
Beyond FPA



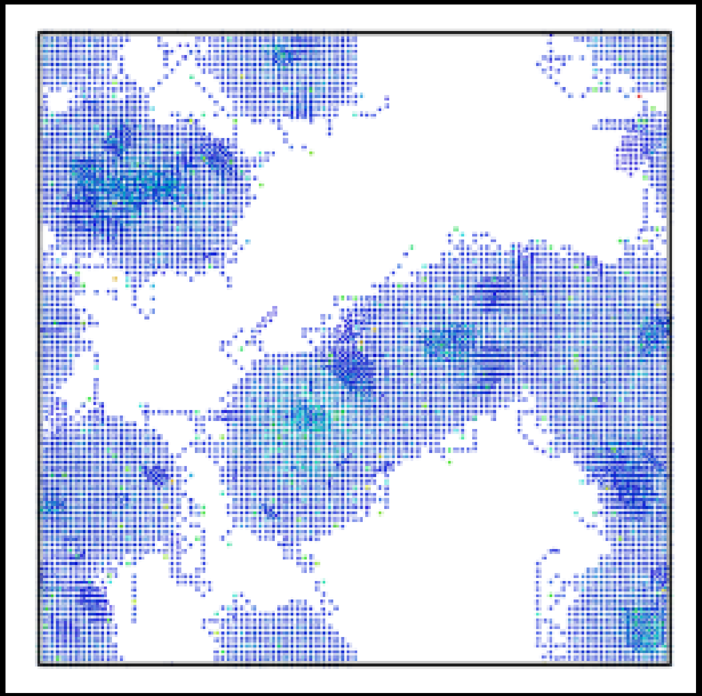




4 cascades



8 cascades

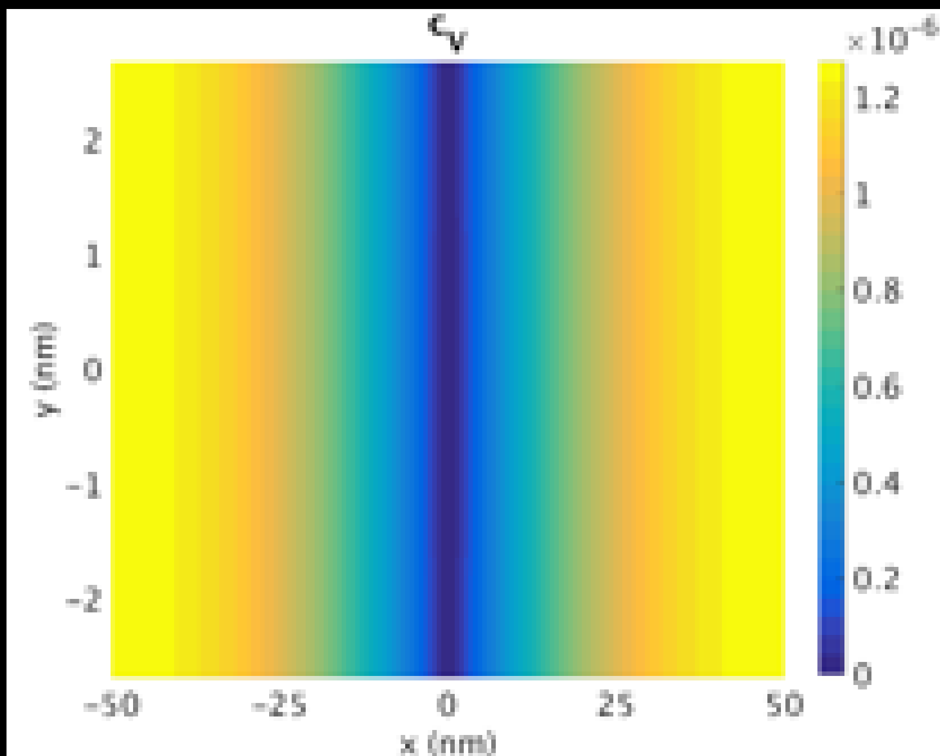


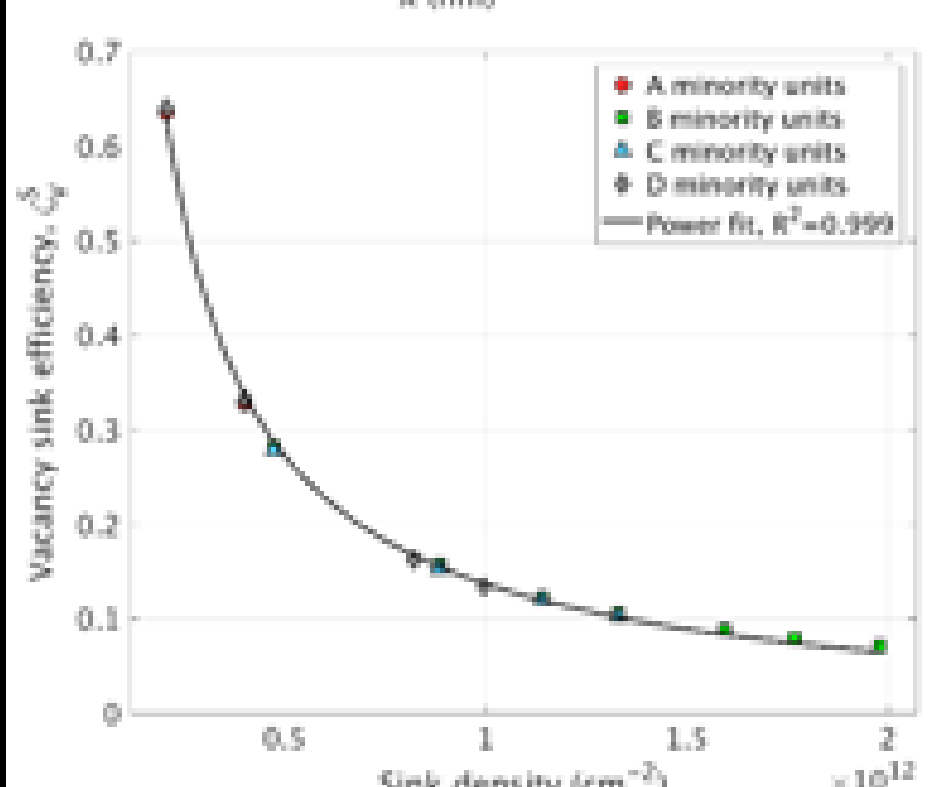
12 cascades

Rapid Assessment of Defect Management at Grain Boundaries and Triple Junctions

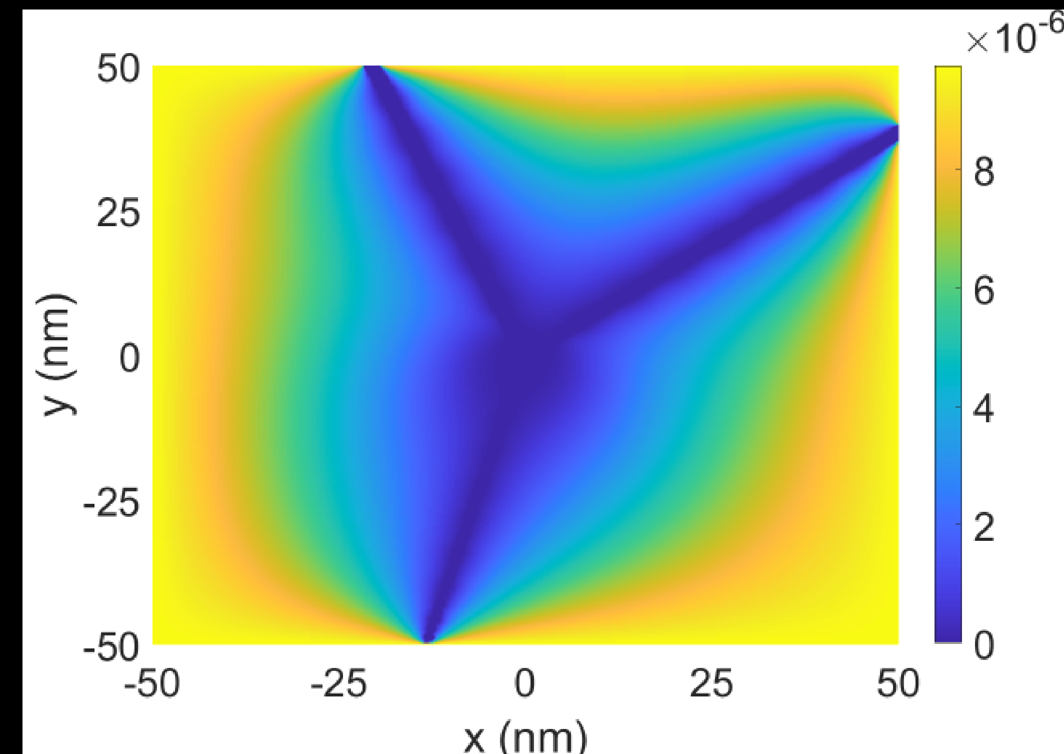
Sandia National Laboratories

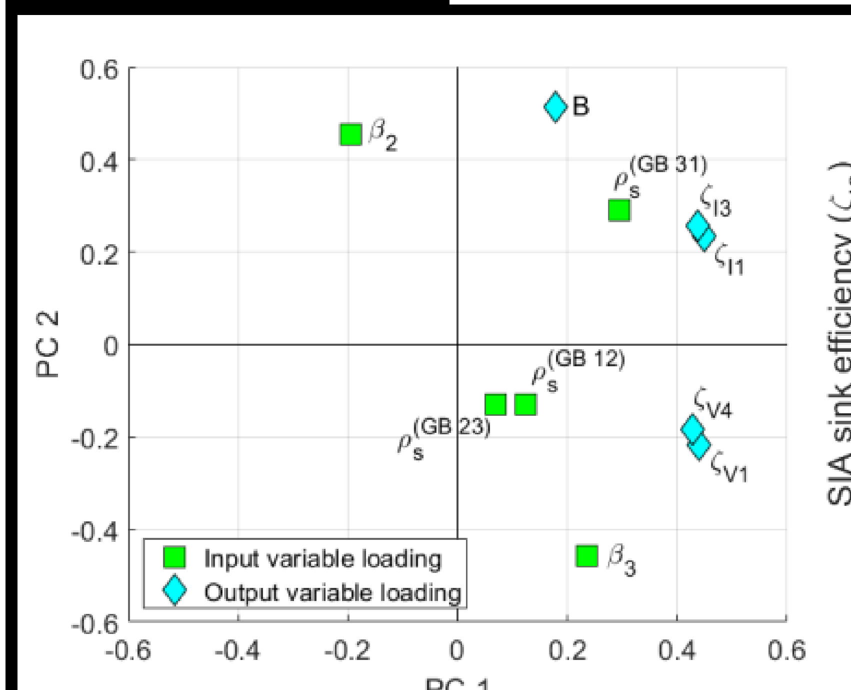
Defect behavior in the vicinity of grain boundaries

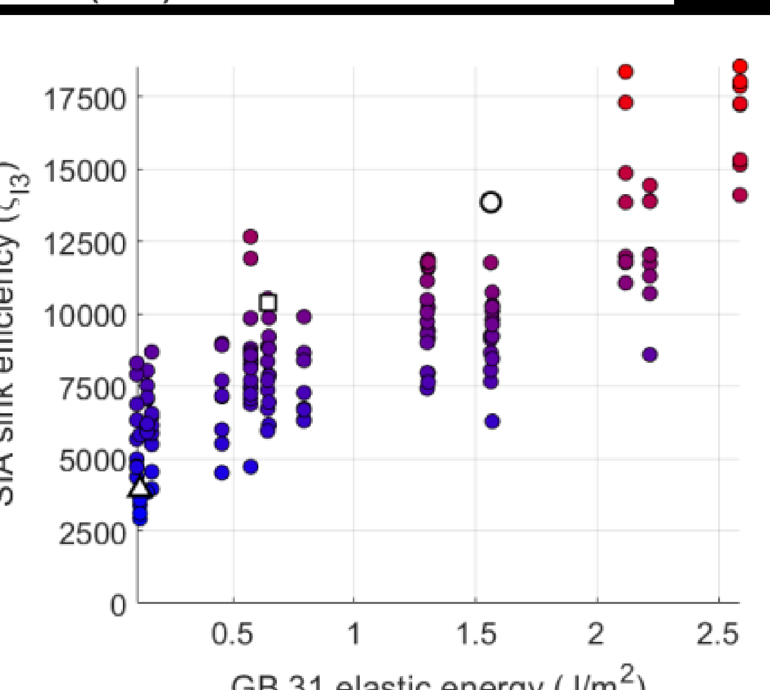




Defect behavior in the vicinity of triple junctions

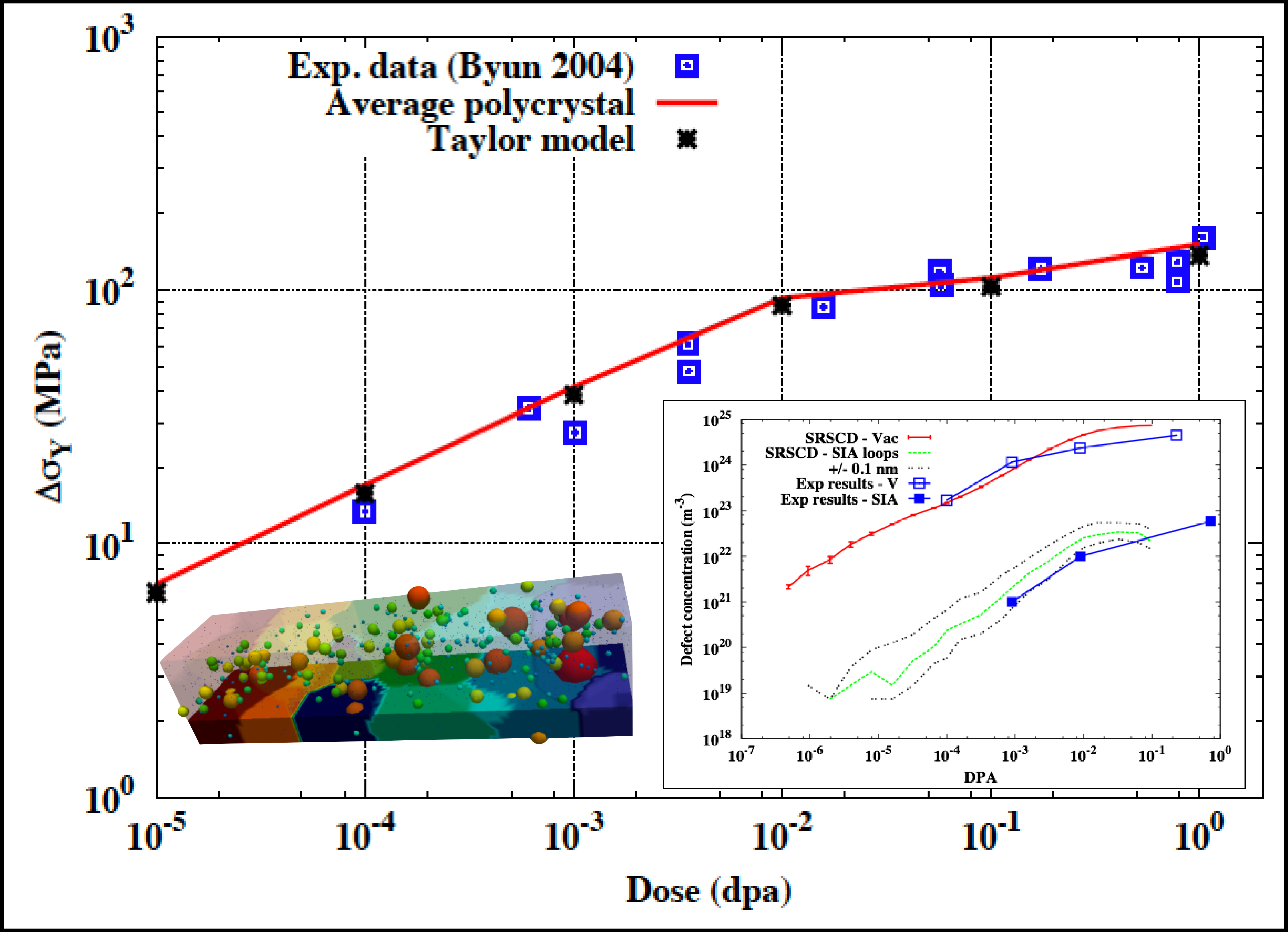






[Zarnas et al. (2018) *Comput. Mater. Sci.*]

Radiation Damage in Nanostructured Materials



[Dunn et al. (2016) *Modell. Simul. Mater. Sci. Eng.*]

NCE!

ATIONAL USER FACILITY FOR NANOSCIENCE

CINT IN NUMBERS

- 4 science thrusts
  - **Nanomechanics**
  - Nanophotonics & optical
  - Quantum nanomaterials
  - Soft, bio nanomaterials
- 2 facilities (SNL/LANL)
- 51 staff scientists
- 32+ postdocs and grad students
- 500+ users
- 200+ projects
- 250+ publications/year
- $0, no fee for pre-competitive research
- 100% full recovery cost for proprietary research

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osal cycle in September…

STUDYING DEFECT-MICROSTRUCTURE INTERACTIONS THROUGH MESOSCALE MODELS

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Long term evolution of defects (concentration and size) beyond what can be achieved using atomistic models

$$\frac{dC_i}{dt} = \sum_{\mu=1}^{M_i} \pm a_\mu^i \left(c_1, \ldots, c_N\right)$$

Reaction	Description
Clustering reactions	
$V_n + V_m \to V_{n+m}$	3D diff, spheres
$V_n + I_m \to V_{n-m}$ or I_{m-n}	3D diff, spheres
$V_n + I_m \to V_{n-m}$ or I_{m-n}	V: 3D diff, sphere; SIA: 1D diff, loop
$I_n + I_m \to I_{n+m}$	3D+3D diff, spheres
$I_n + I_m \to I_{n+m}$	3D+1D diff, sphere + loop
$I_n + I_m \to I_{n+m}$	1D+1D diff, loops
Dissociation reactions	
$V_n \to V + V_{n-1}$	V cluster: sphere
$I_n \to I + I_{n-1}$	I cluster: sphere
$I_n \to I + I_{n-1}$	I cluster: loop
Migration reactions	
$X^i \to X^j$	(cell i to cell j)
Implantation reactions	
$0 \to V + I$	Frenkel pair
$0 \to (cascade)$	Cascade

Clustering

$$V_n + V_m \to V_{m+n}:$$

$$\text{reaction rate} = \omega\left(n^{1/3} + m^{1/3}\right)\left(D_{V_n} + D_{V_m}\right) C_{V_n}(t) C_{V_m}(t)$$

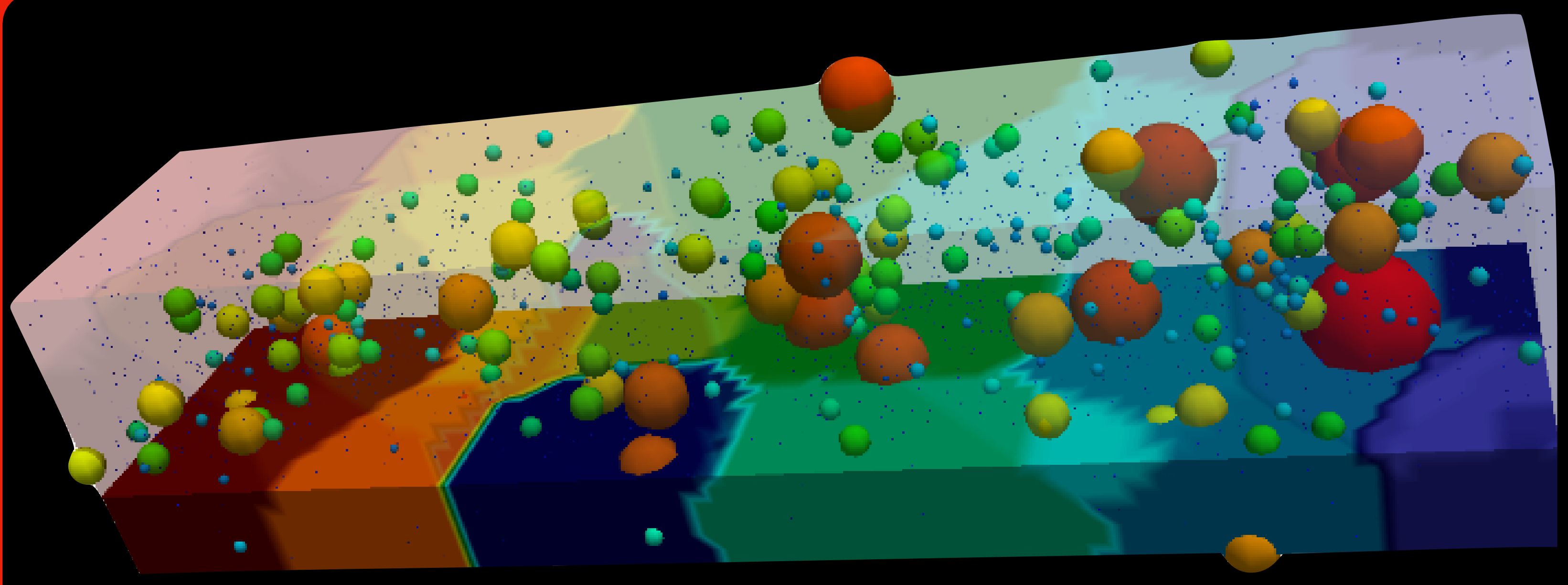
Dissociation

$$V_n \to V_{n-1} V_1:$$

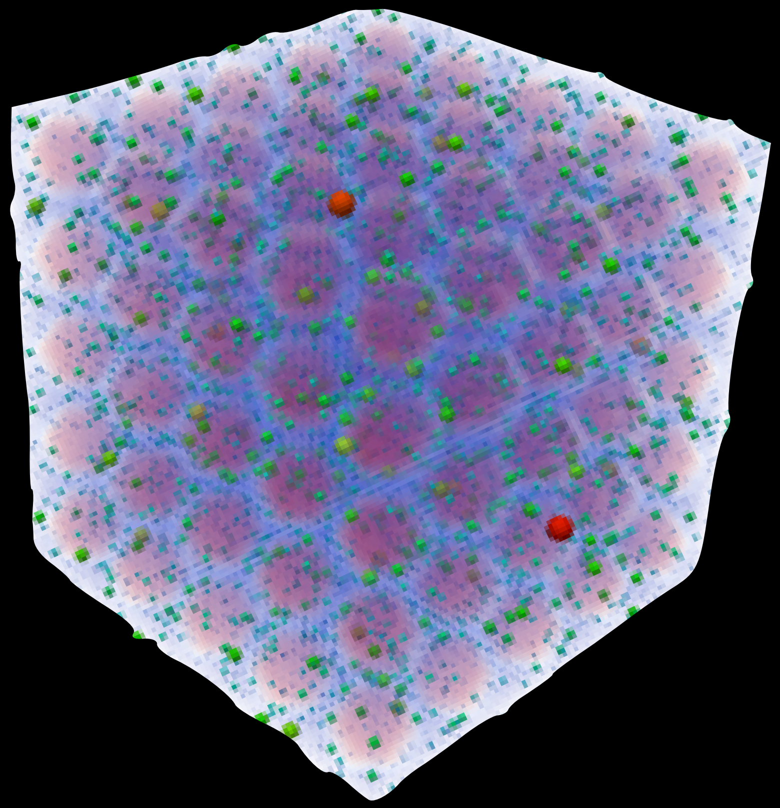
$$\text{reaction rate} = \omega n^{1/3} D_{V_n} \exp\left(\frac{-E_b}{k_b T}\right) C_{V_n}(t)$$

Collaboration with A. Dunn (GaTech), L. Capolungo (LANL), C. Hin (VaTech), P. Zarnas (NW), J. Qu (Tufts)

Radiation Damage in Nanostructured Materials



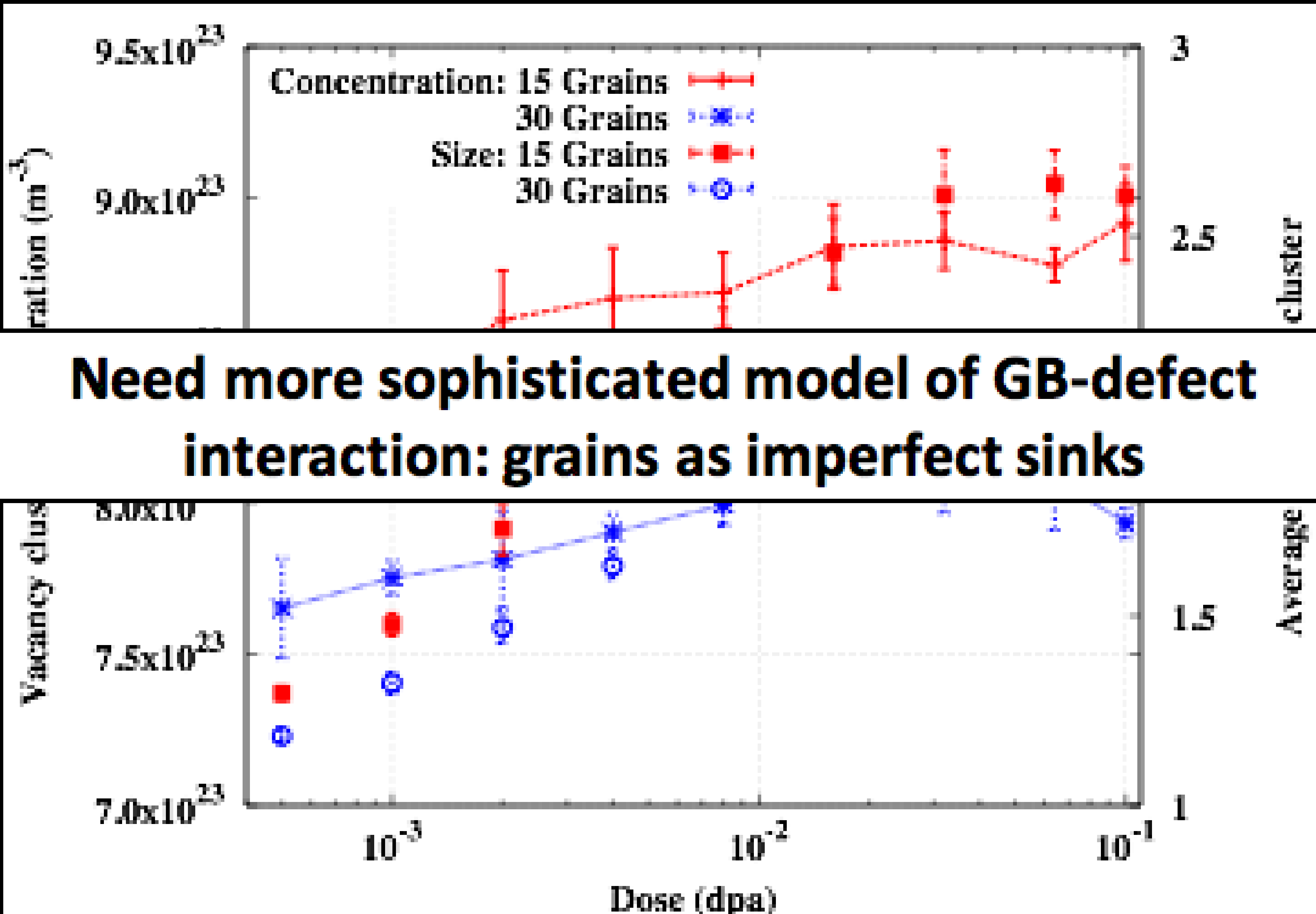
Nanocrystalline



Nanoporous

[Dunn et al. (2016) *Modell. Simul. Mater. Sci. Eng.*]

Radiation Damage in Nanostructured Materials



Need more sophisticated model of GB-defect interaction: grains as imperfect sinks

[Dunn et al. (2016) *Modell. Simul. Mater. Sci. Eng.*]