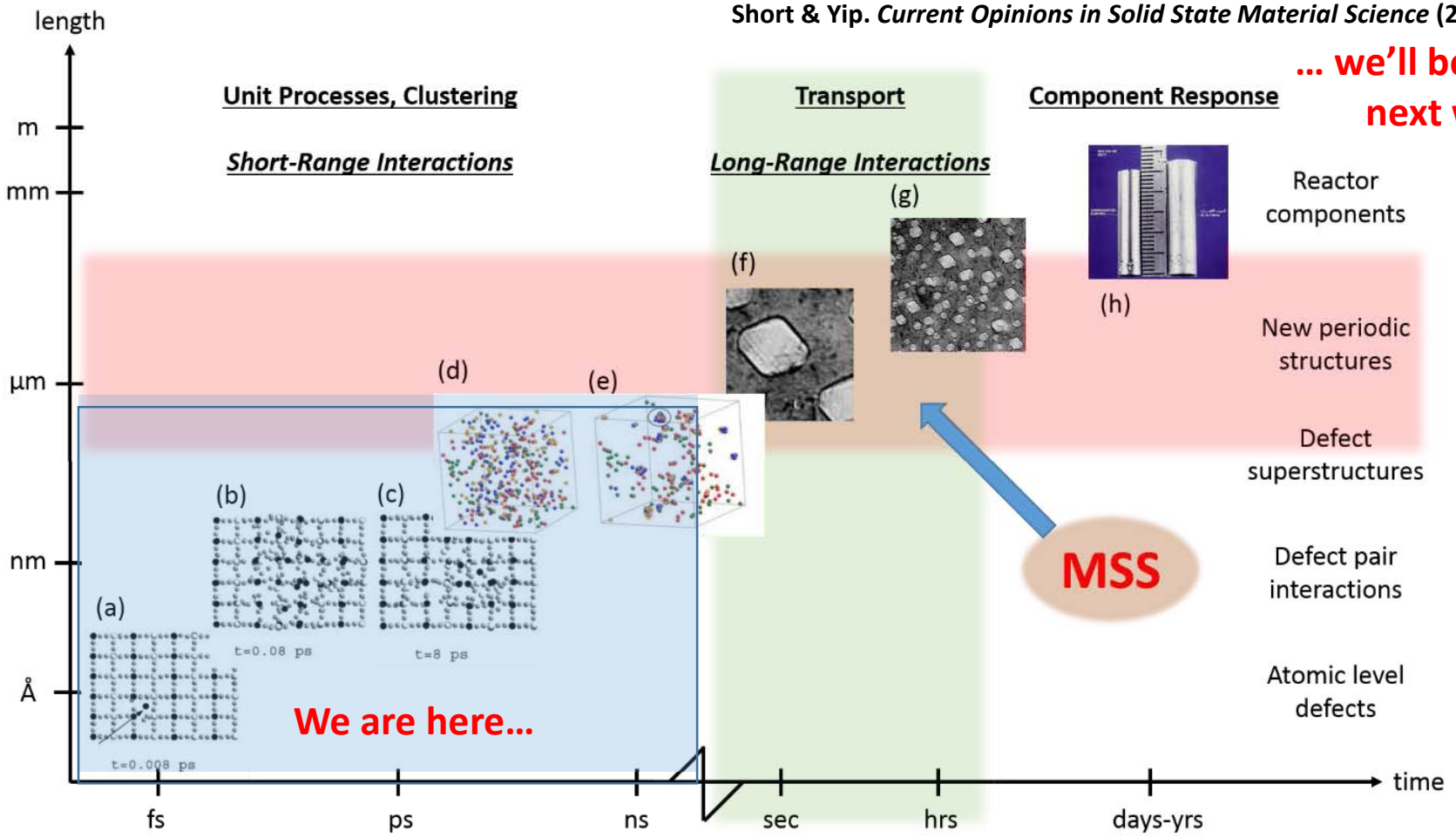
Radiation Stopping Power, Damage Cascades, Displacement and the DPA

Learning Objectives

- Predict stopping power of radiation as functions of material, type, energy of radiation
- Conceptualize radiation damage cascades, stages, and evolution in time
- Estimate the quantitative displacement rates from radiation, and define the DPA
- Track the buildup of radiation point defects as functions of temperature, defect concentration

Building Up to Radiation Effects

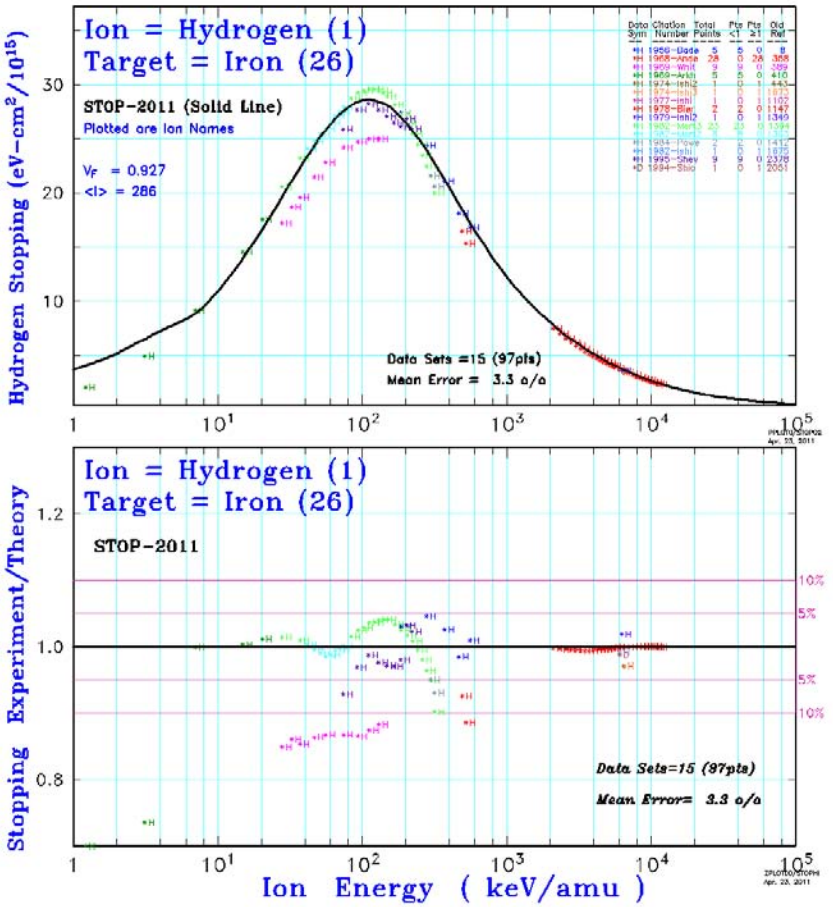


Source: Short, M., and S. Yip. "Materials Aging at the Mesoscale: Kinetics of Thermal, Stress, Radiation Activations." *Current Opinion in Solid State and Materials Science* 19, no. 4 (2015): 245-52.

Stopping Power

http://www.srim.org

- More energetic particles do more damage … to a point
- … but how much?
- Charge vs. no charge?
- What about damage vs. mean free path?



Courtesy of James F. Ziegler. Used with permission.

Stopping power of protons in iron

Coulombic/Nuclear Stopping Power

- *Stopping Power* is defined as differential energy loss as a function of energy:

$$N * S(E) = -\frac{\partial E}{\partial x}$$

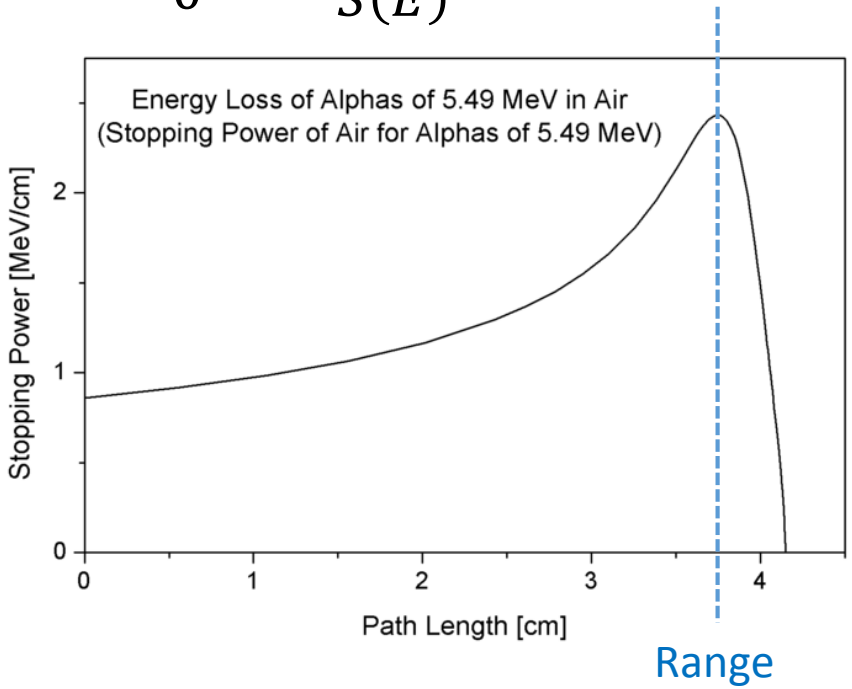
- Separable components due to nuclear (screened nucleus Coulombic), electronic, and radiative terms:

$$N * S(E) = -\left(\frac{\partial E}{\partial x}\right)_{nucl.} - \left(\frac{\partial E}{\partial x}\right)_{elec.} - \left(\frac{\partial E}{\partial x}\right)_{rad.}$$

Range

Source: Wikimedia Commons

- Integrate inverse of stopping power over the energy range of the particle: $Range = \int_0^{E_{max}} \frac{1}{S(E)} dE$
- Not all particles have identical range, *straggling* describes this variation



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Stopping Power Components

H. Paul. *AIP Conf. Proc.* 1525:309 (2013)

- Nuclear stopping power: First assume Coulombic nucleus interactions, describe interatomic potential:

$$V(r) = \frac{Z_1 Z_2 \varepsilon^2}{r} \quad \text{(1/r dependence)}$$

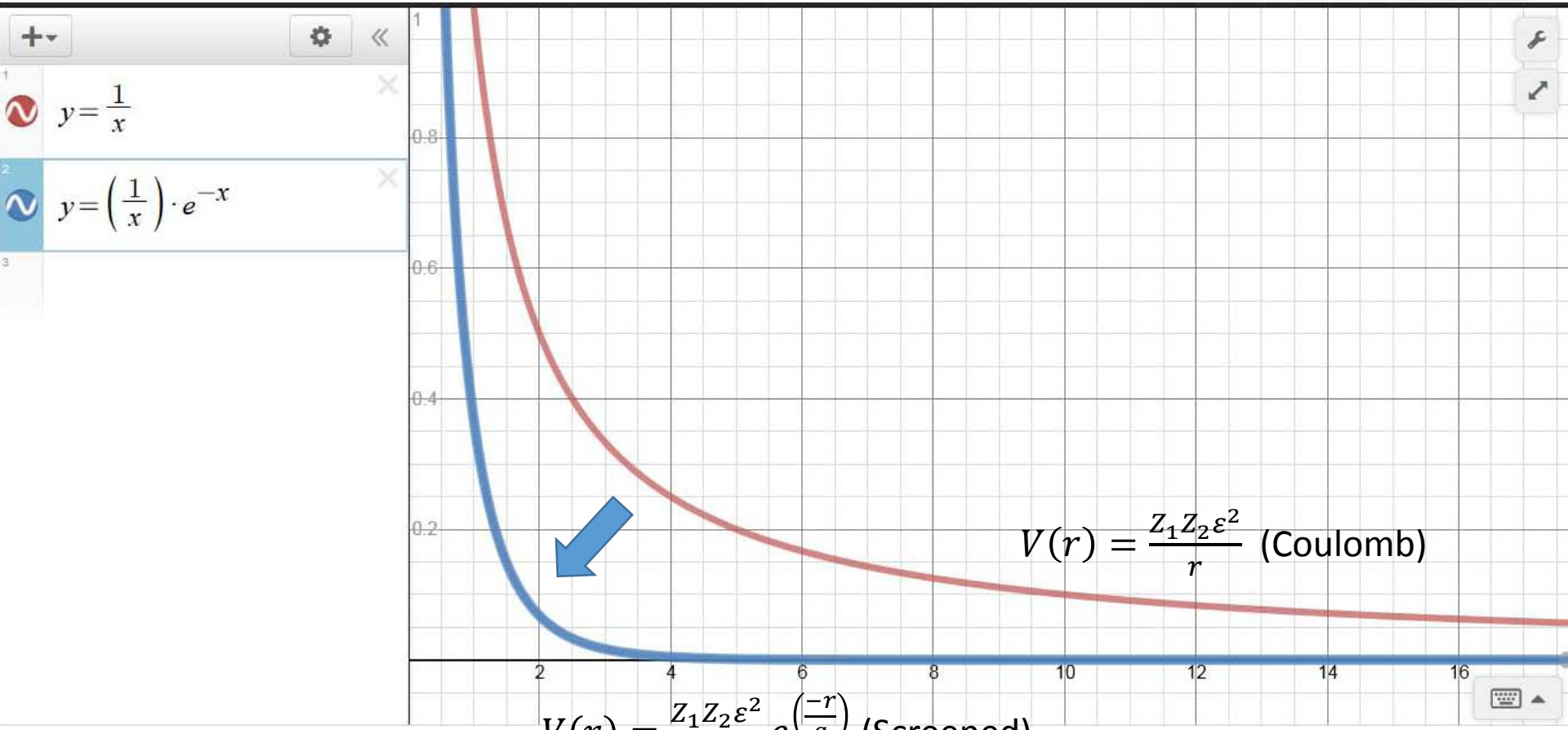
- Positive nucleus screened by negative electron cloud:

$$V(r) = \frac{Z_1 Z_2 \varepsilon^2}{4\pi\varepsilon_0 r} e^{\left(\frac{-r}{a}\right)}$$

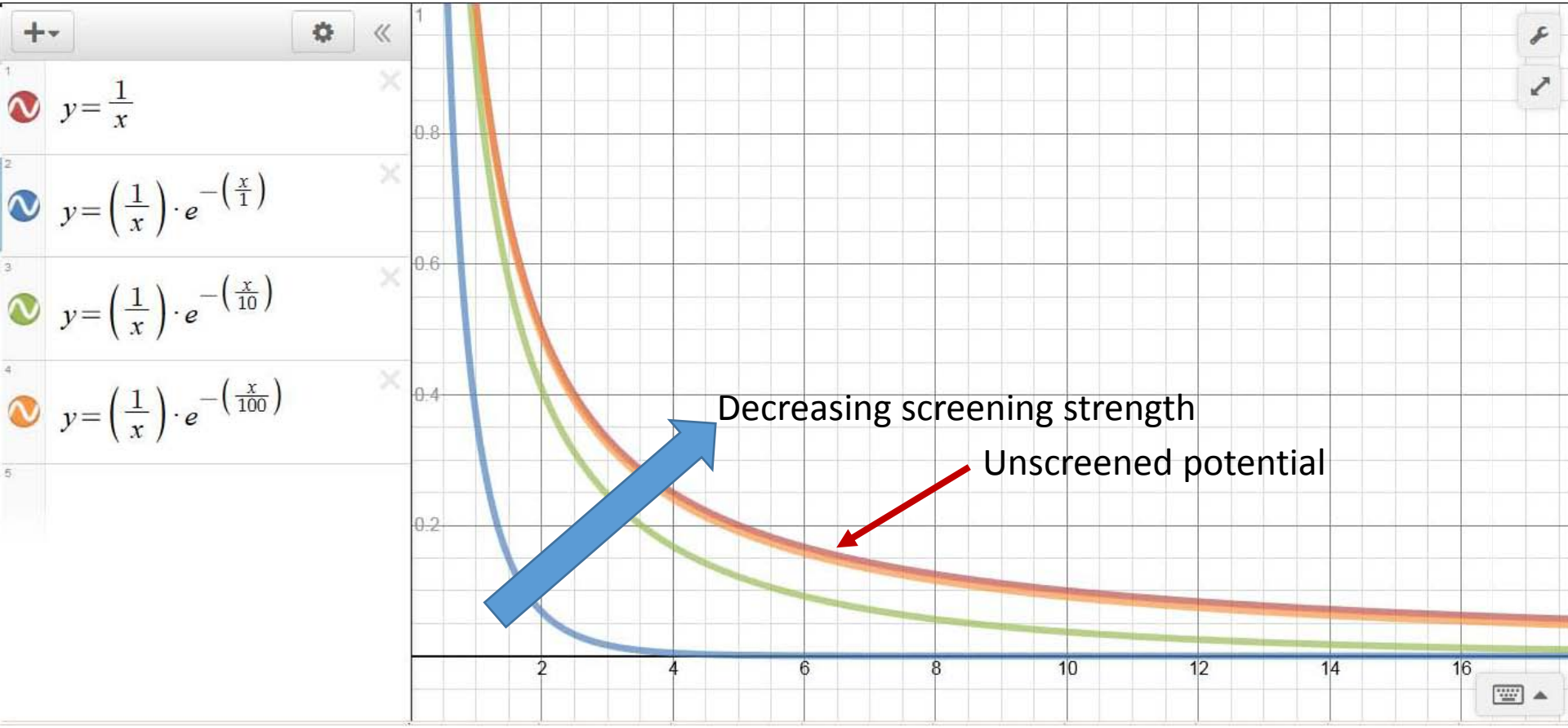
Effective screening radius

Stopping Power Components

Pretty graphs by Desmos Grapher (www.desmos.org)



Stopping Power Components



Stopping Power Components

- Assume $\left(\frac{dE}{dx}\right)_{rad.} \approx 0$

$$\gamma = \frac{4mM}{(m+M)^2}$$

- Nuclear stopping power formula (Was p. 47):

$$\left(\frac{dE}{dx}\right)_{nucl.} = \frac{N\pi Z_1 Z_2 \varepsilon^4}{E_i}\frac{M_1}{M_2}\ln\left(\frac{\gamma E_i}{\frac{\varepsilon^2 \gamma E_a^2}{4E_i}}\right)$$

$$\left(\frac{dE}{dx}\right)_{nucl.} = \frac{N\pi Z_1 Z_2 \varepsilon^4}{E_i}\frac{M_1}{M_2}\ln\left(\frac{4E_i^2}{\varepsilon^2 E_a^2}\right)$$

Stopping Power Components

- Now turn to electronic stopping. The Bethe-Bloch formula describes this well:

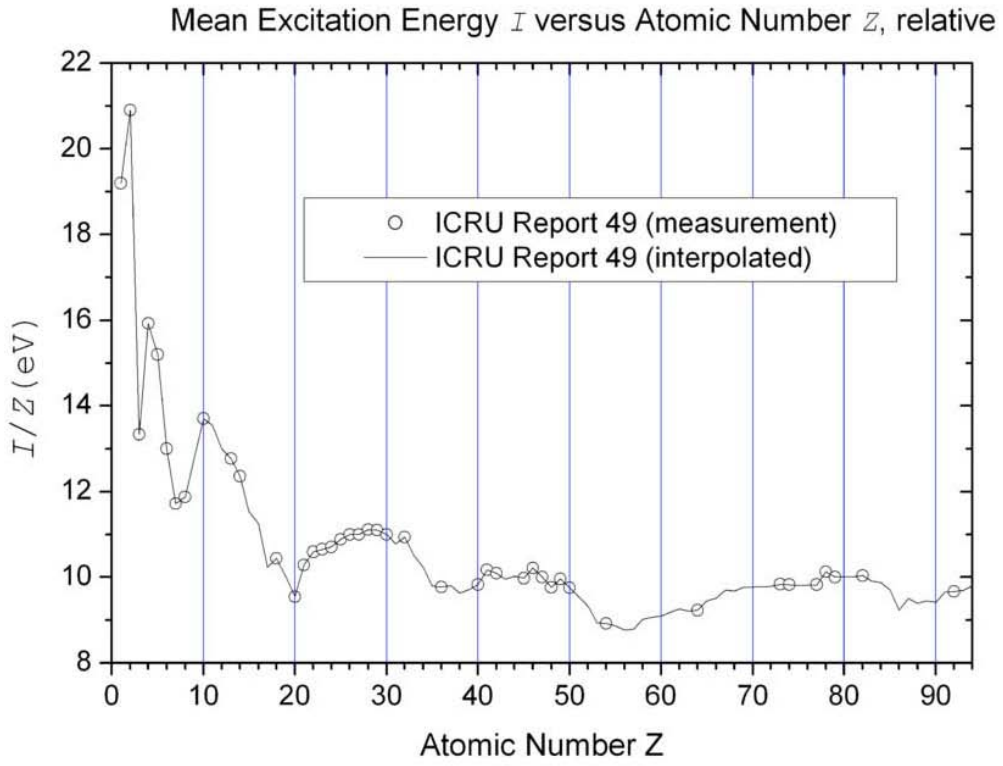
$$-\left(\frac{dE}{dx}\right) = \frac{4\pi k_0^2 Z^2 \varepsilon^4 n_e}{m_e c^2 \beta^2}\left[\ln\left(\frac{2m_e c^2 \beta^2}{I(1-\beta^2)}\right) - \beta^2\right]$$

$$\beta = \frac{v_{ion}}{c}; \quad n_e = electron\ density$$

- I is the mean excitation energy of the medium

Stopping Power Components

- *I* is the mean excitation energy of the medium



Relative Stopping Powers

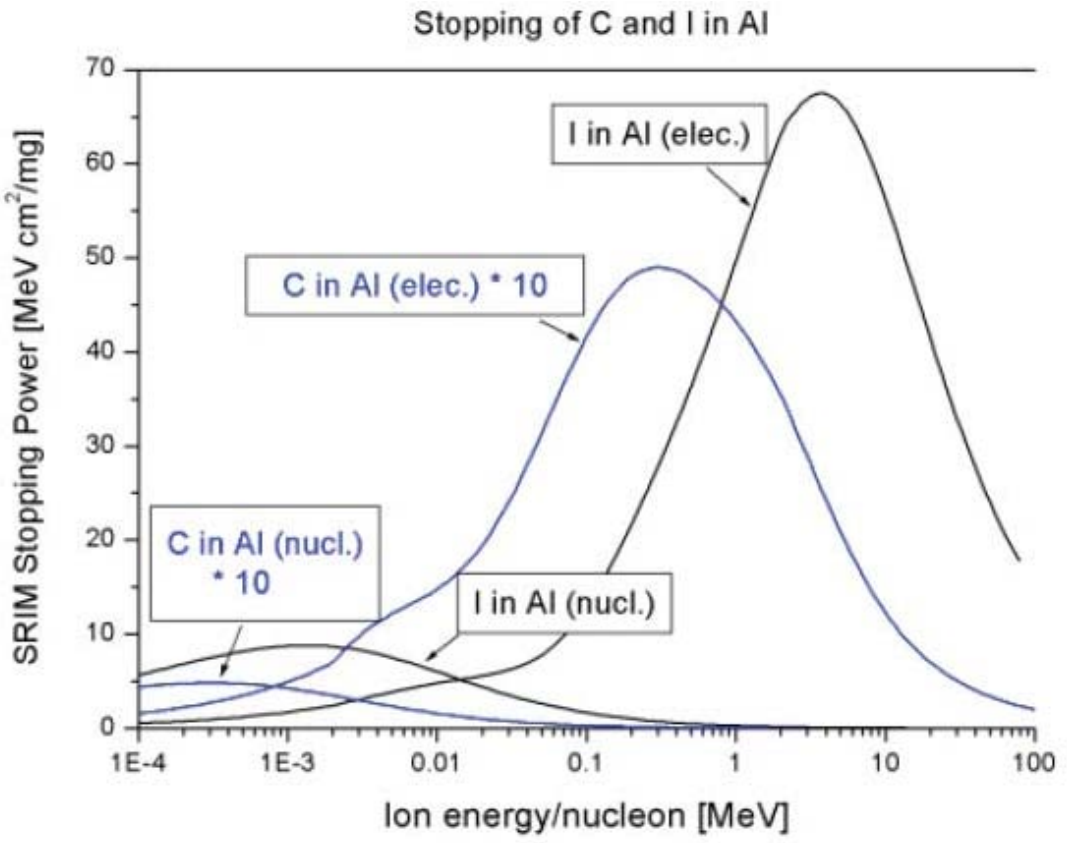
- Plot/compare S_e/S_n

$$\frac{S_e}{S_n} = \frac{2M_2}{m_e Z_2} \frac{\ln\left(\frac{\gamma_e E_i}{I}\right)}{\ln\left(\frac{\gamma E_i}{E_d}\right)}$$

- Electronic stopping power takes over by factors of 10^2-10^4 for high energy ions…
- … what about neutrons?

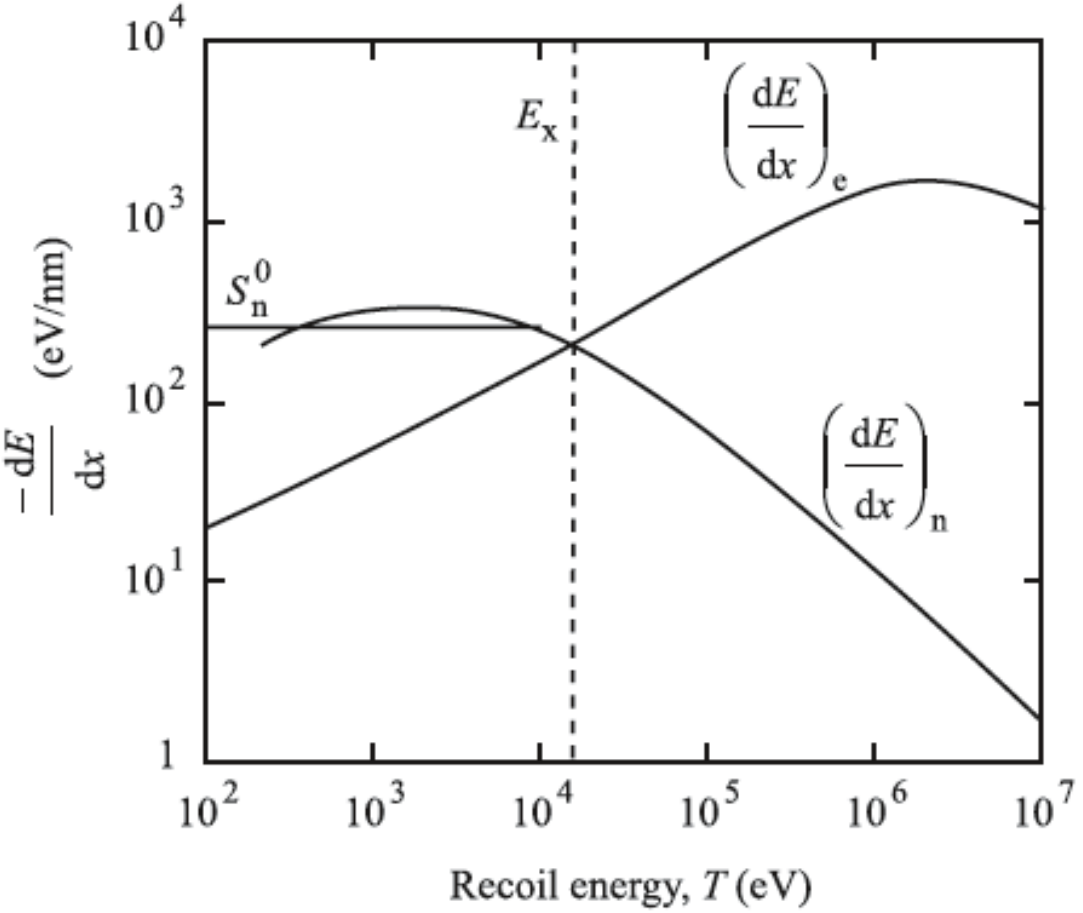
Relative Stopping Powers

H. Paul. *AIP Conf. Proc.* 1525:309 (2013)



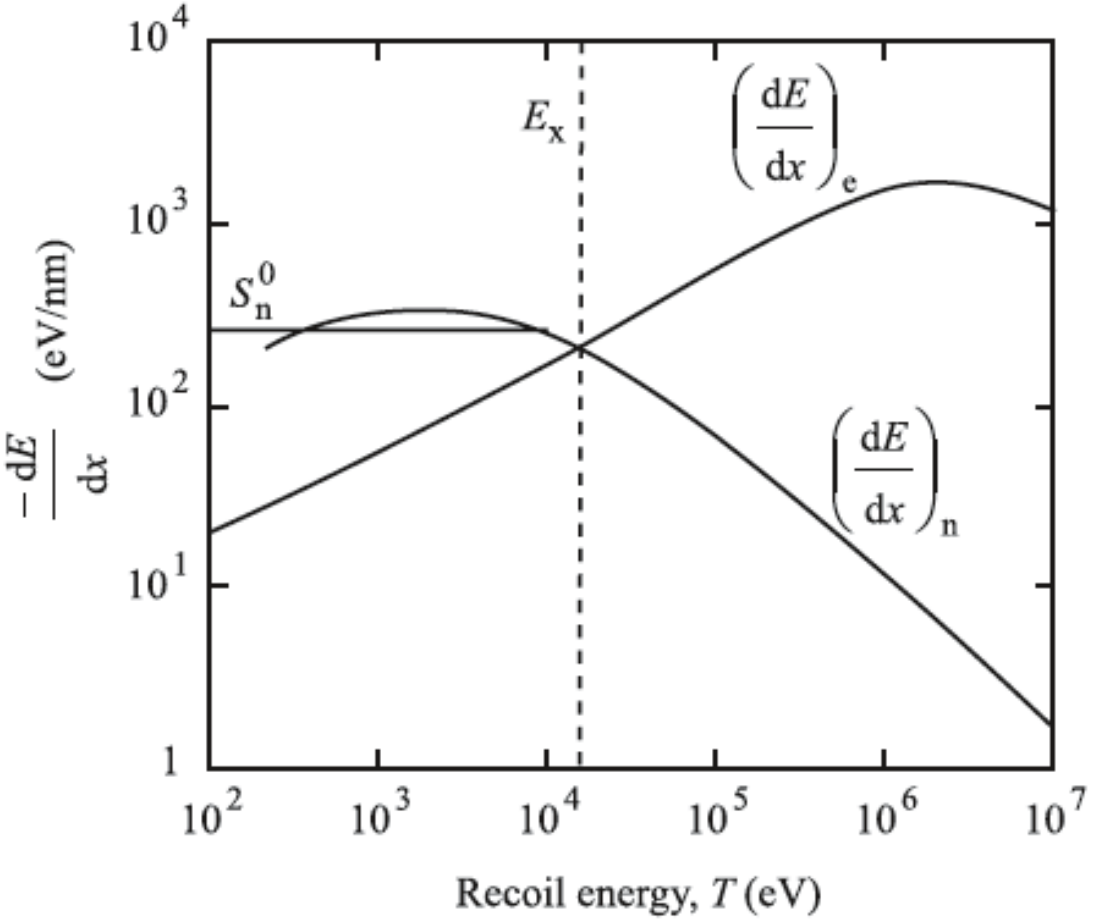
Relative Stopping Powers

Was, p. 84



Relative Stopping Powers

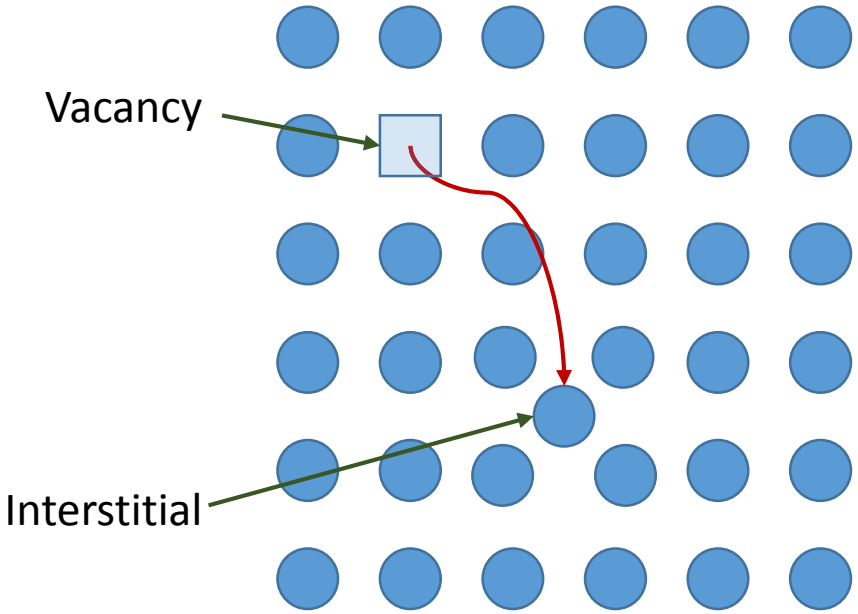
Was, p. 84



- What does this say about:
  - Energy deposition vs. energy at high-E?
  - Same at low-E?
- When is the most damage done to a material?
- Explain damage rates vs. ranges of heavy ions & fast neutrons?
- …
- What about thermal neutrons?

It All Starts with Frenkel Pairs

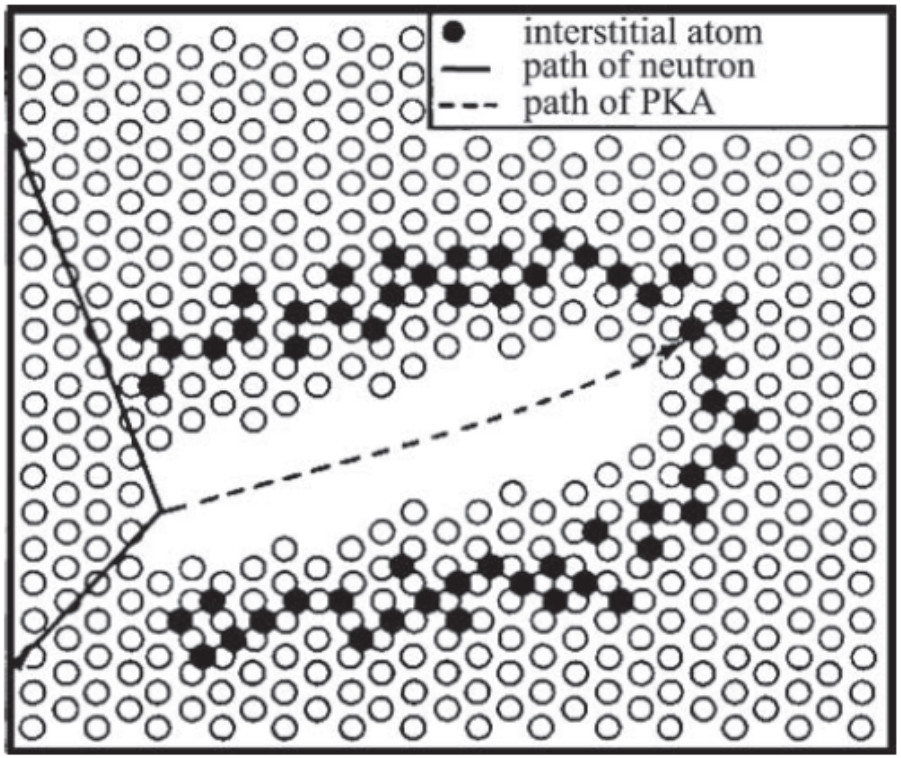
- Frenkel pair – perfect vacancy/interstitial combination
- Produced very well by electron radiation



The Damage Cascade

Was, p. 128

- Frenkel pairs don't stay that way!
- Many ideas about how "damage cascade" evolves
  - Called "cascade" due to subsequent, continuing damage effects
- What's wrong with this picture?

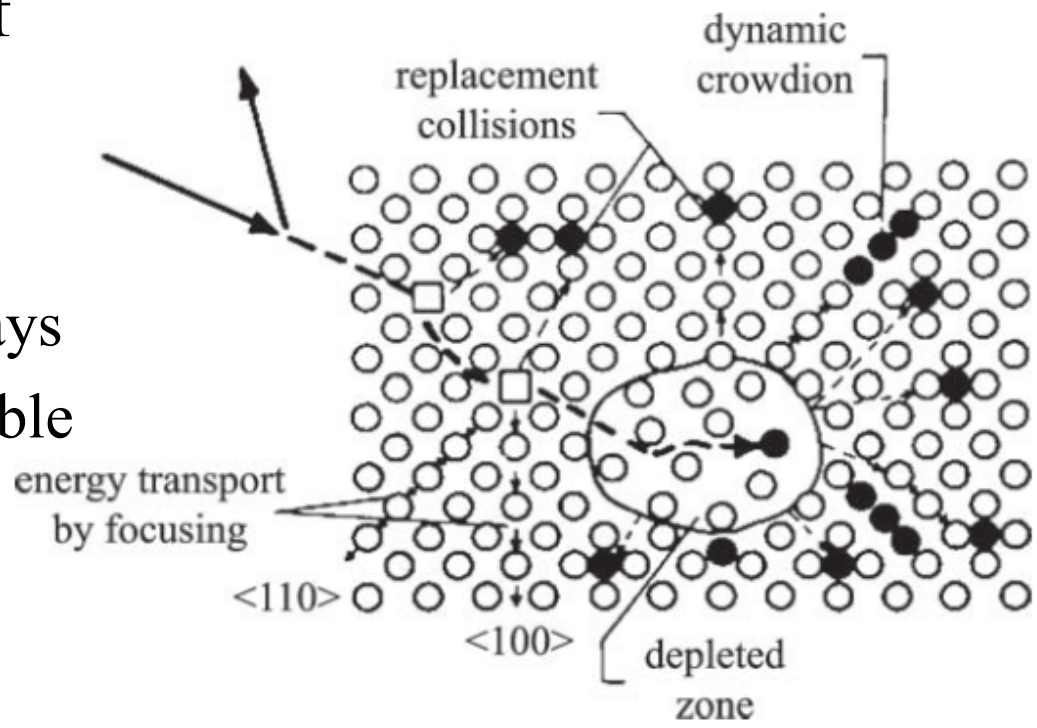


Original conception of damage cascade, showing path of Frenkel pair production

Damage Cascades Revisited

Was, p. 128

- Many more forms of damage are possible
  - Single vacancies & interstitials not always energetically favorable
  - Frenkel pairs don't explain observed damage



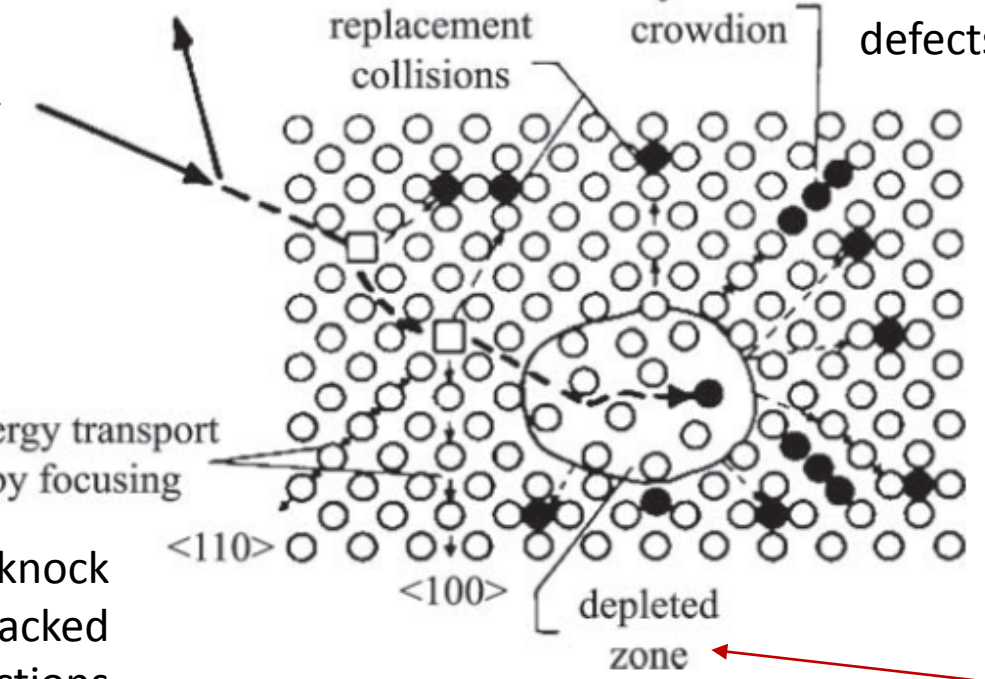
Revised damage cascade accounting for crystallinity

Damage Cascades Revisited

Was, p. 128

Stable, energetically favorable, fast-moving defects

Primary Knock-on Atom (PKA)

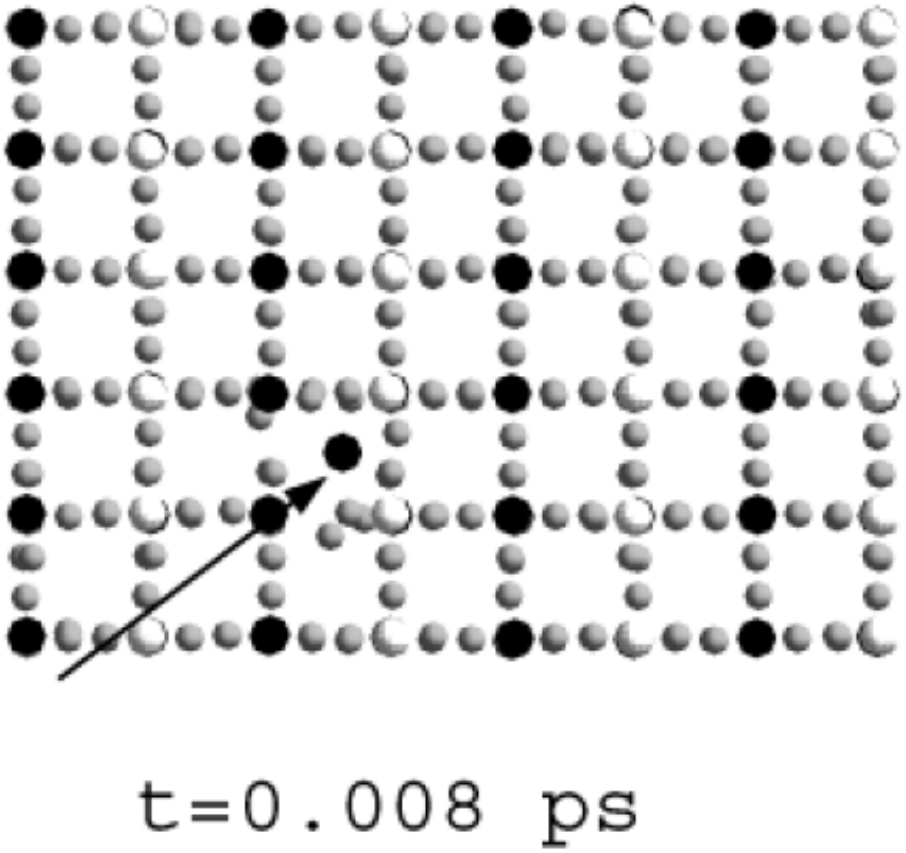


Collisions can knock atoms in close-packed directions

How stable would this be in the long term?

Cascade Stages – Ballistics

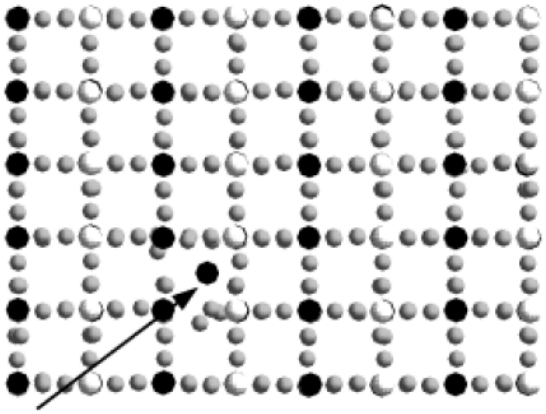
- Put simply, atoms get knocked around
- No time to relax!
- ~10MeV neutrons move how fast?
  - How long to move one lattice parameter?



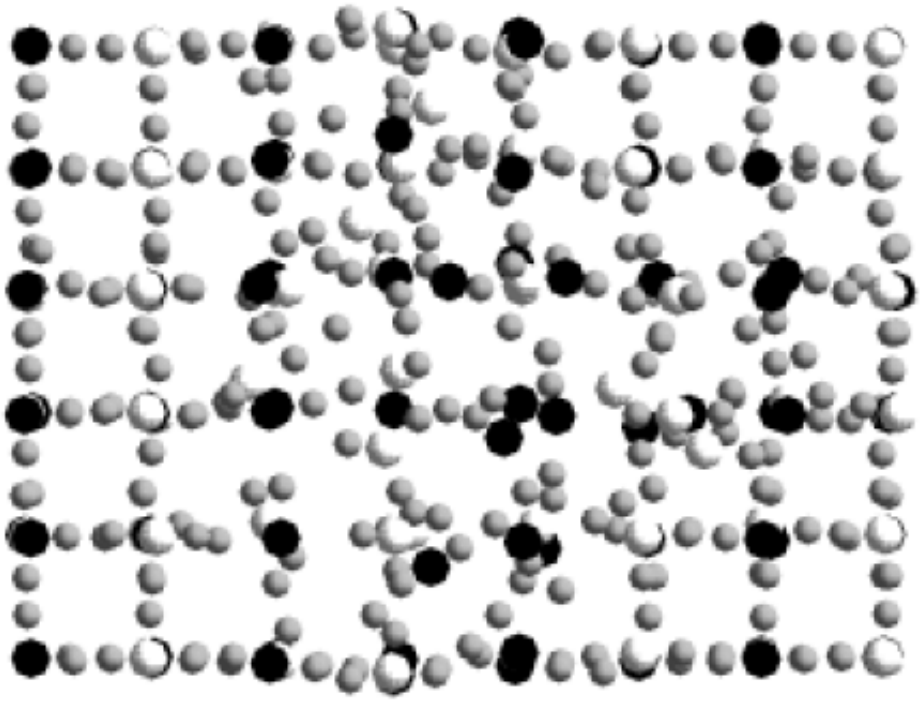
K. O. Trachenko, M. T. Dove. E. K. H. Salje. *J. Phys. Condens. Matter*, 13:1947 (2001)

Cascade Stages – Thermal Spike

- Temperature rises very locally for a very short time



t=0.008 ps

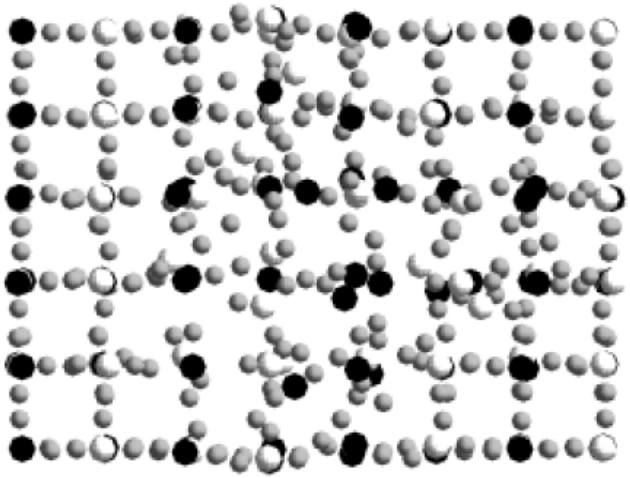


t=0.08 ps

K. O. Trachenko, M. T. Dove. E. K. H. Salje. *J. Phys. Condens. Matter*, 13:1947 (2001)

Cascade Stages – Quench

- Heat is conducted away EXTREMELY quickly



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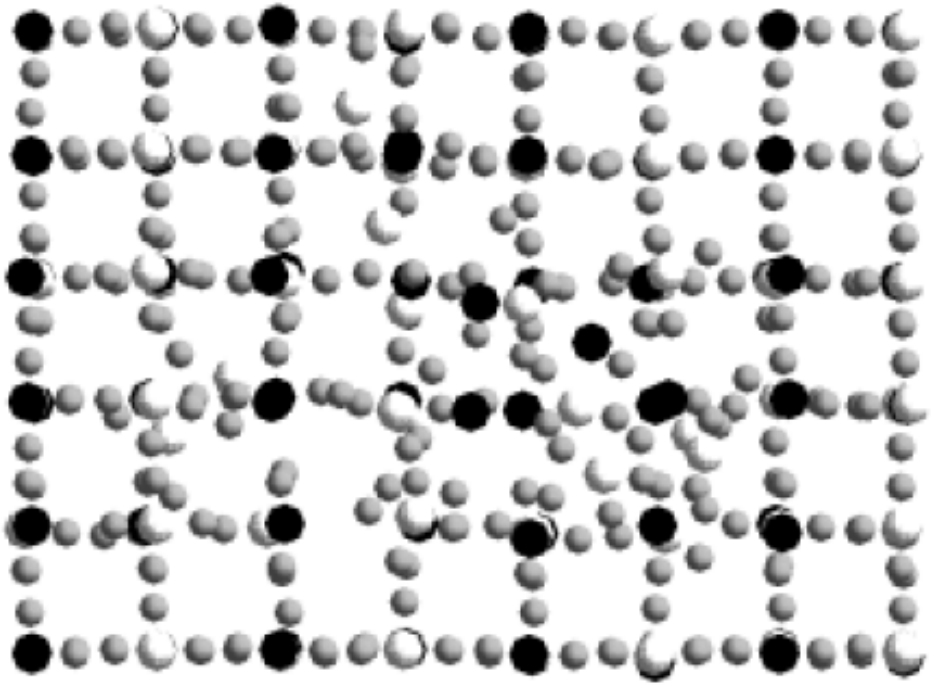


t=8 ps

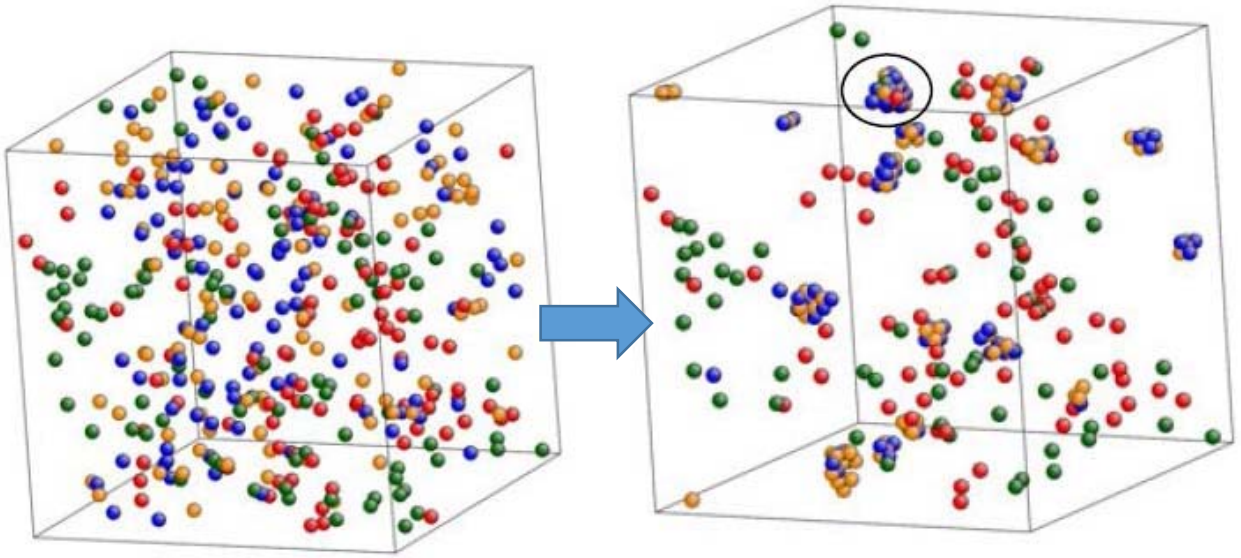
K. O. Trachenko, M. T. Dove. E. K. H. Salje. *J. Phys. Cond. Matter*, 13:1947 (2001)

Cascade Stages – Anneal

D. S. Aidhy et al. *Scripta Mater.*, 60(8):691 (2009)

- Most damage "anneals" out, or recombines/gets sunk away
  - For neutrons & ions, *almost all* damage anneals!

$t = 0\ ns$

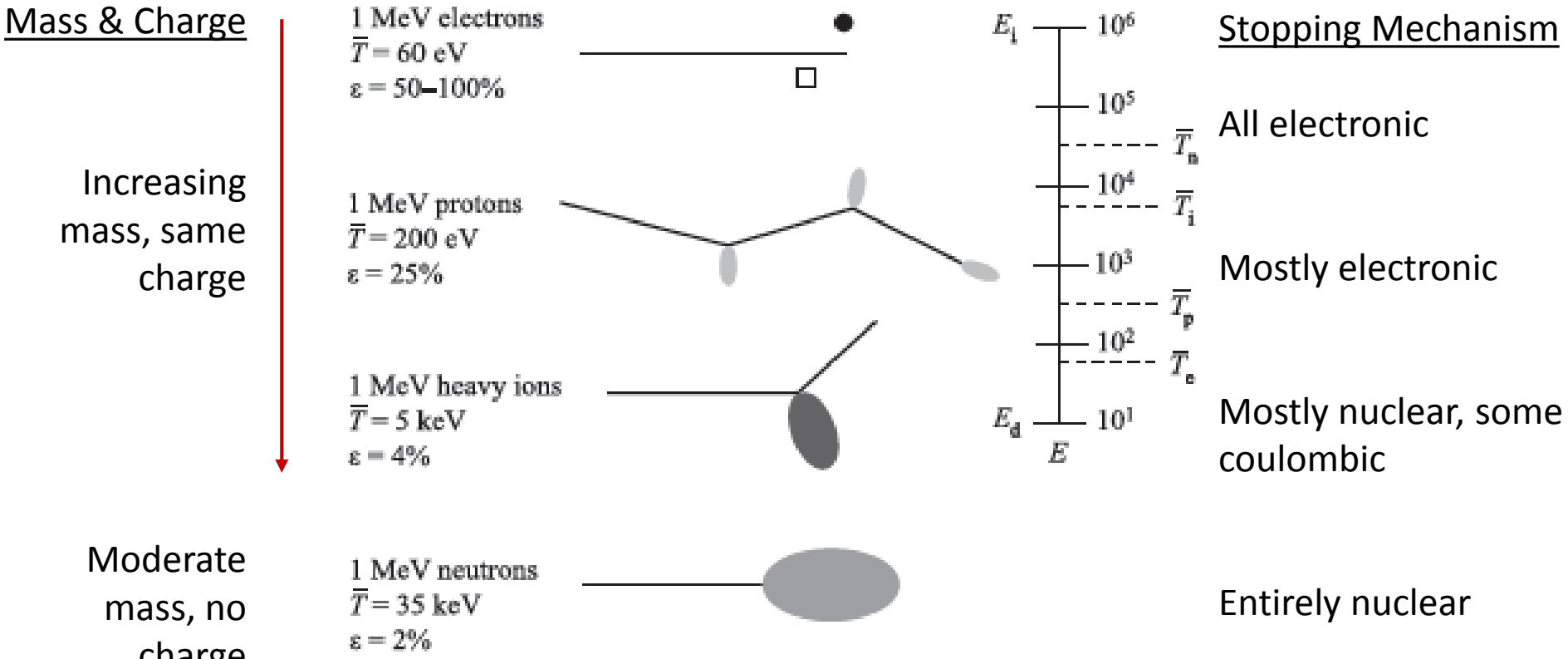


$t = 2.45\ ns$

Simulated annealing of Frenkel pairs in MgO at 1000K

Types of Radiation

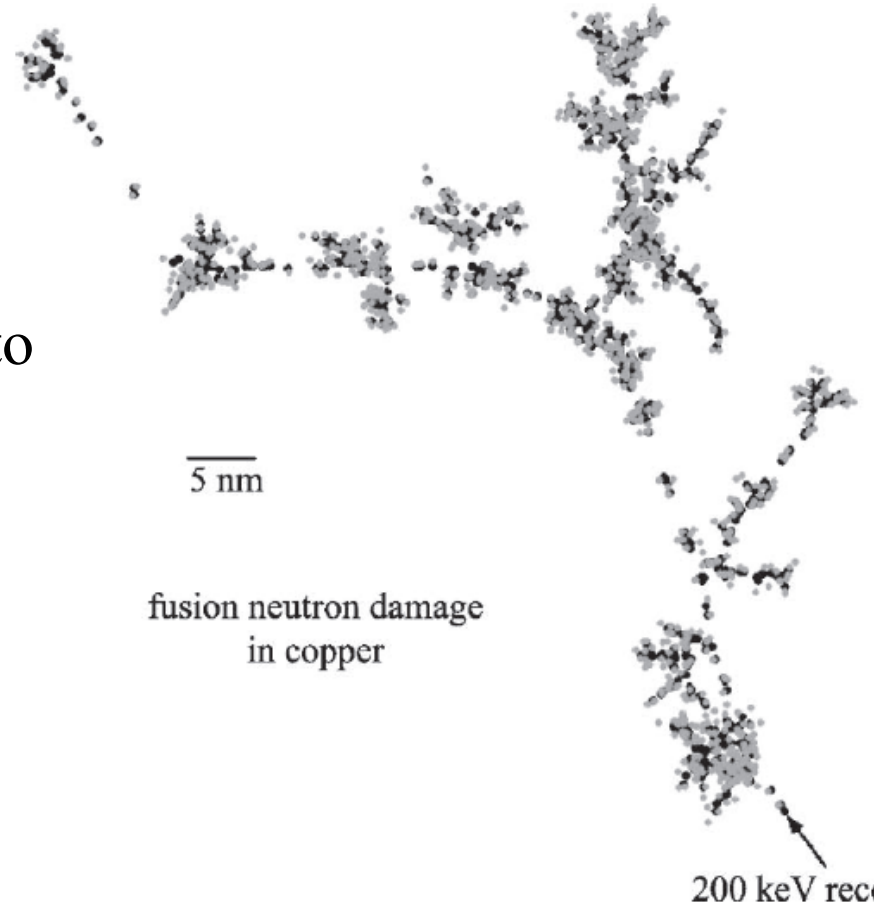
- Different radiation produces different cascades



Simulation Methods – BCA

Was, p. 134

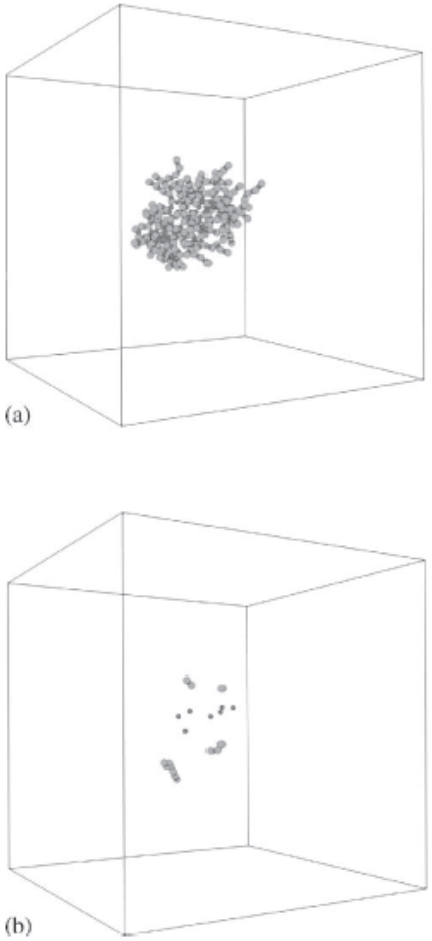
- Binary Collision Approximation
  - Uses interatomic potentials (like MD) to allow atoms to move
  - Does not restrict crystallinity
  - Creates collision cascades pretty well!



Simulation Methods – MD

Was, p. 139

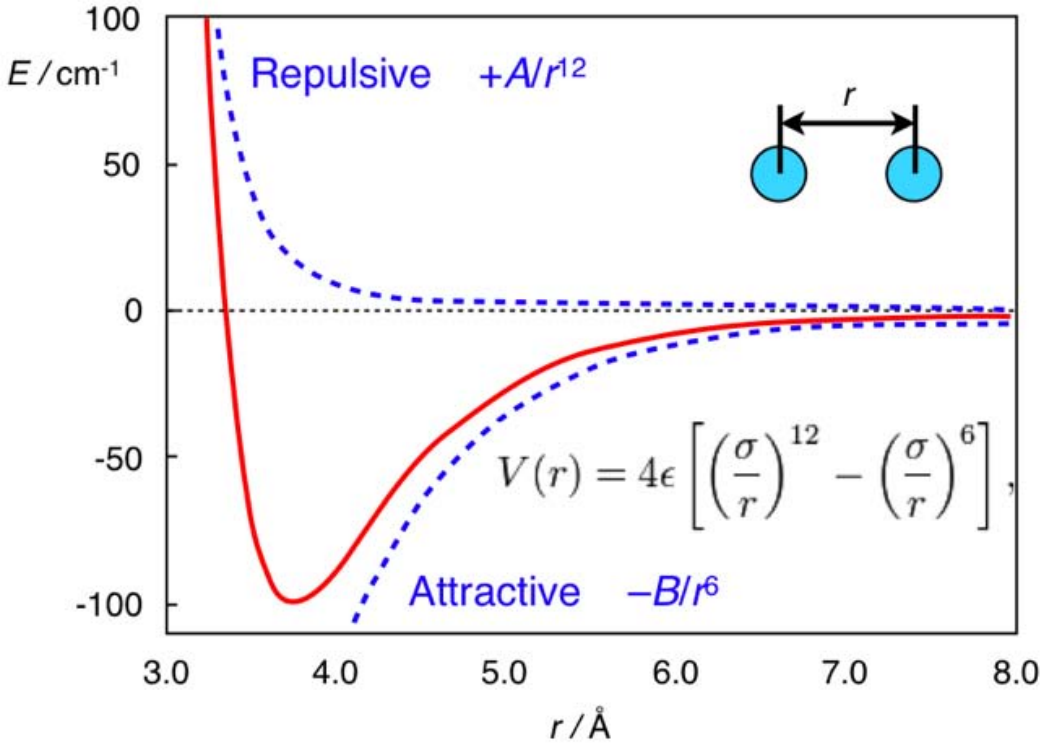
- Solve $F = ma$ for every pair of atoms
- *Interatomic potentials* are the key to interactions
  - *Right:* MD simulation of 1keV cascade in iron at 100K



Simulation Methods – MD

http://www.cmbi.ru.nl/redock/images/LennardJones.png

- *Interatomic potentials* are the key to interactions
- Attractive & repulsive terms
  - **Lennard-Jones (LJ) potential** widely used



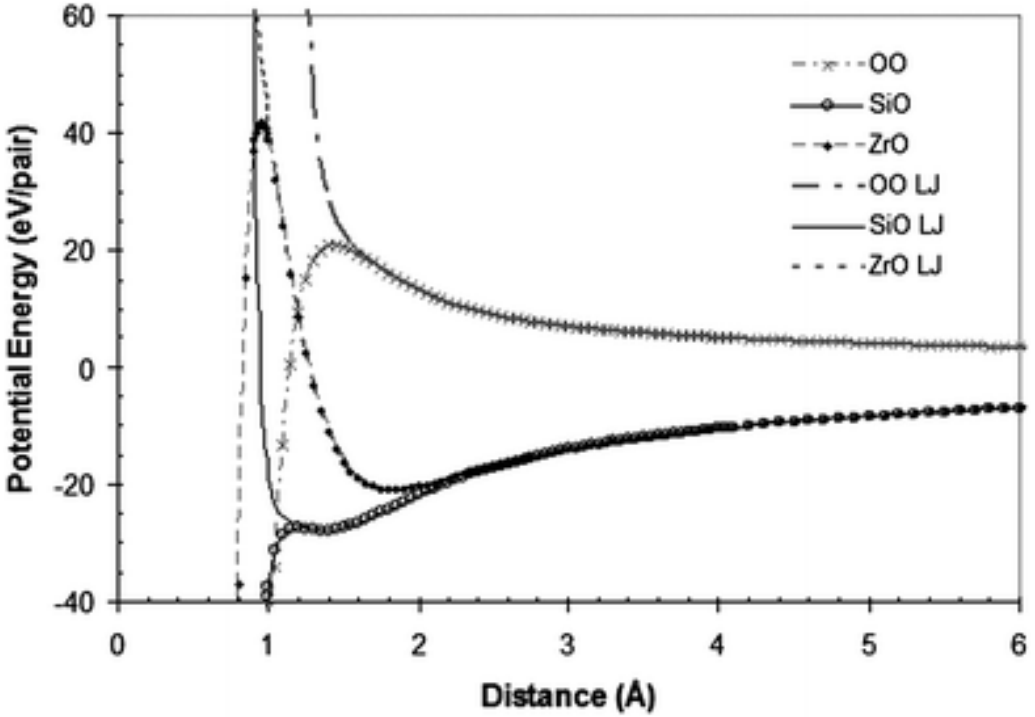
Courtesy of Bo Hanssen & Sander Jans. Used with permission.

Lennard-Jones Potential

Simulation Methods – MD

J. Yu et al. *J. Mater. Chem.*,19:3923-3930 (2009)

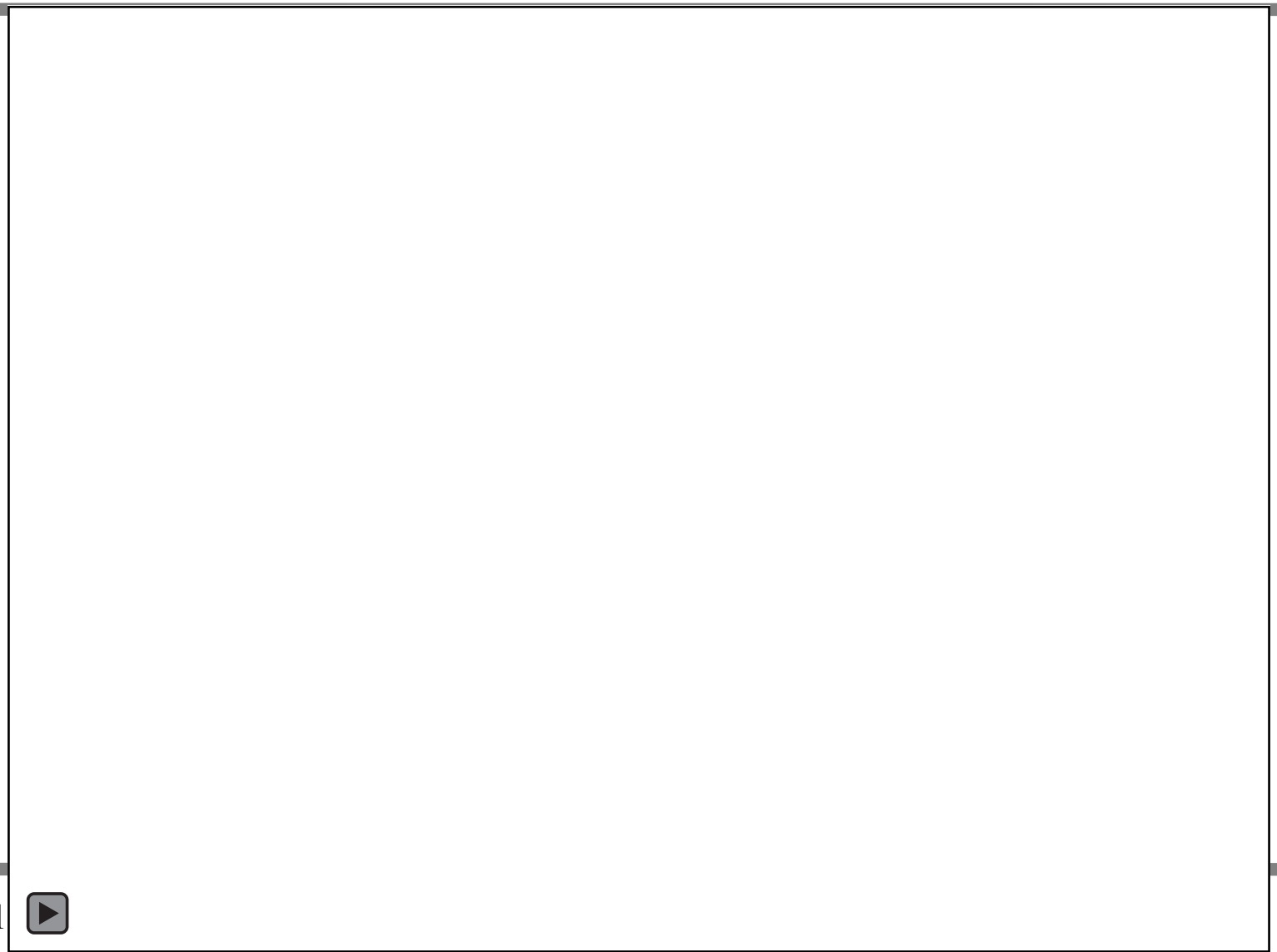
- *Interatomic potentials* are the key to interactions
- Attractive & repulsive terms
  - Lennard-Jones (LJ) potential widely used



Attractive terms of selected potentials (dots), and LJ-modified version (lines)

Simulation Methods – MD

A video is played in class to demonstrate the concept. http://www-personal.umich.edu/~gsw/movies.html



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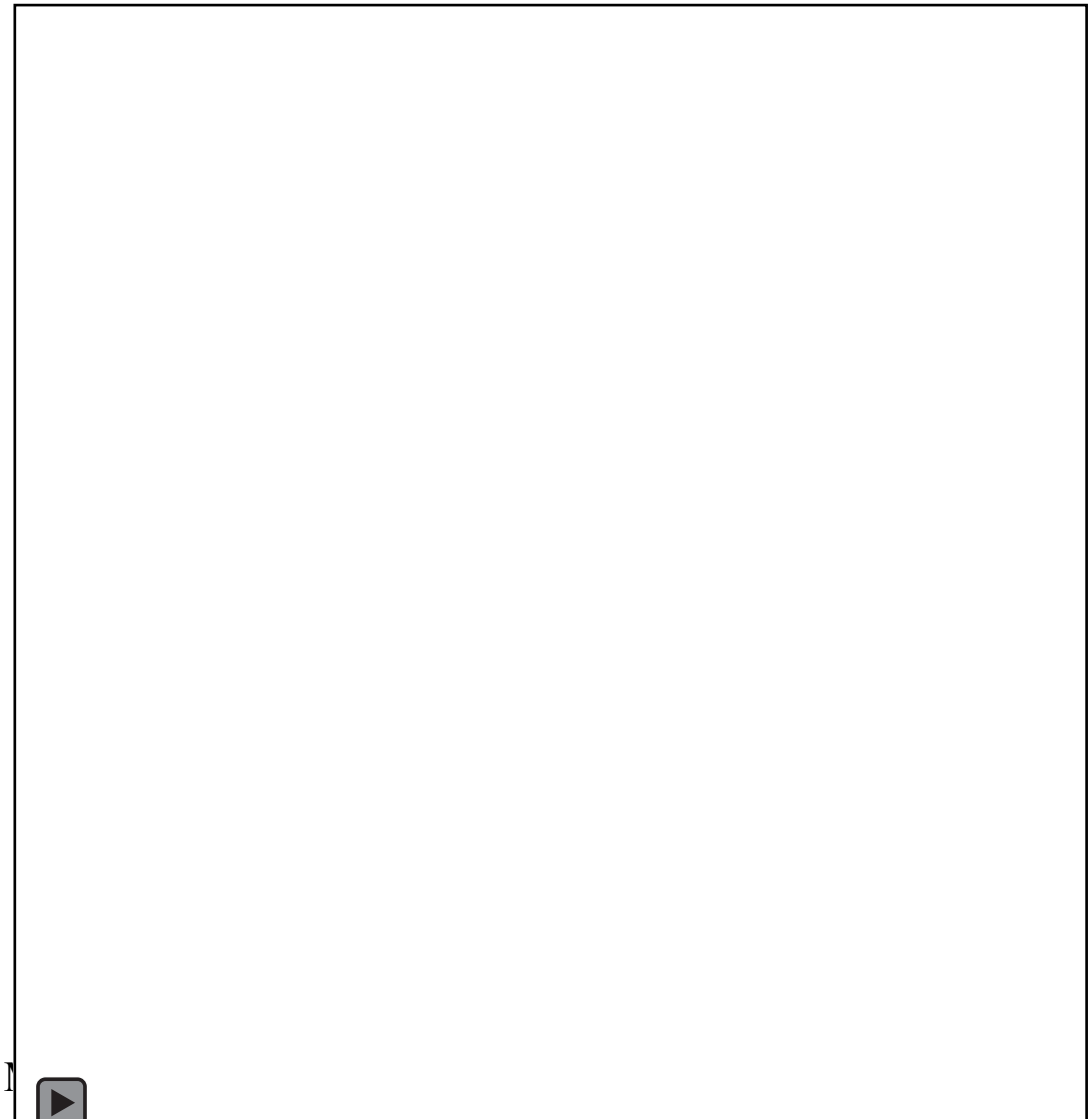
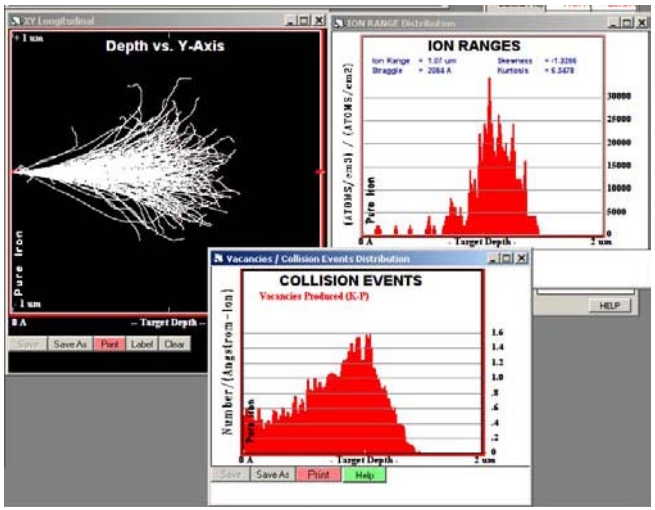


Simulation Methods – MC

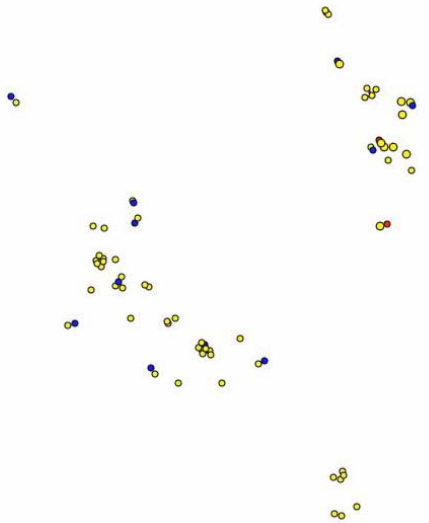
- With pre-determined distributions for some features
  - "Roll the dice" to sample from distributions
  - Let random numbers determine where things move and change
- Example: TRIM
  - Randomly choose scattering angles, new mean free paths



Simulation Methods – MC

http://www-personal.umich.edu/~gsw/movies.html

3.2 Kinetic Monte Carlo (KMC) simulation of a 20 keV cascade in Fe-0.2Cu-0.6Si-0.7Ni-12.4Mn steel (similar to a reactor pressure vessel steel) at 327°C. The simulation shows the enrichment of nickel (green atoms), Mn (black atoms), Si (blue atoms) and Cu (red atoms) at vacancy clusters (in yellow) covering a time period out to ~0.007 s or about 6-7 orders of magnitude longer than the cascade quench time. Note also the pairing of Ni and Si and the accumulation of solute atoms at the vacancy clusters. (courtesy, C. Becquart, University of Lille)



Simulation Methods – Rate Theory

C. J. Ortiz, M. J. Caturla. J. Computer-Aided Materials Design 14:171-181 (2007)

- Assume rate-controlled equations for defect migration, clustering
- Often employs "mean field theory"
  - Glosses over details to accelerate time

$$\mathrm{I} + \mathrm{V} \rightleftharpoons 0$$
$$\mathrm{V}_n + \mathrm{V} \rightleftharpoons \mathrm{V}_{n+1}$$
$$\mathrm{I}_n + \mathrm{I} \rightleftharpoons \mathrm{I}_{n+1}$$
$$\mathrm{I}_n + \mathrm{I}_2 \rightleftharpoons \mathrm{I}_{n+2}$$
$$\mathrm{I}_n + \mathrm{V} \rightarrow \mathrm{I}_{n-1}$$
$$\mathrm{V}_n + \mathrm{I} \rightarrow \mathrm{V}_{n-1}$$

$$G_X^B(n) = G_X^f + \left(G_X^B(2) - G_X^f\right) \cdot \frac{n^{2/3} - (n-1)^{2/3}}{2^{2/3} - 1}, \quad (7)$$

Table 1 Binding energies of small interstitial and vacancy clusters in Fe according to Fu et al. [9]

	I_n (eV)	V_n (eV)
$n = 2$	0.80	0.30
$n = 3$	0.92	0.37
$n = 4$	1.64	0.62

Simulation Methods – Rate Theory

C. J. Ortiz, M. J. Caturla. J. Computer-Aided Materials Design 14:171-181 (2007)

- How good is the approximation? Is it worth it?

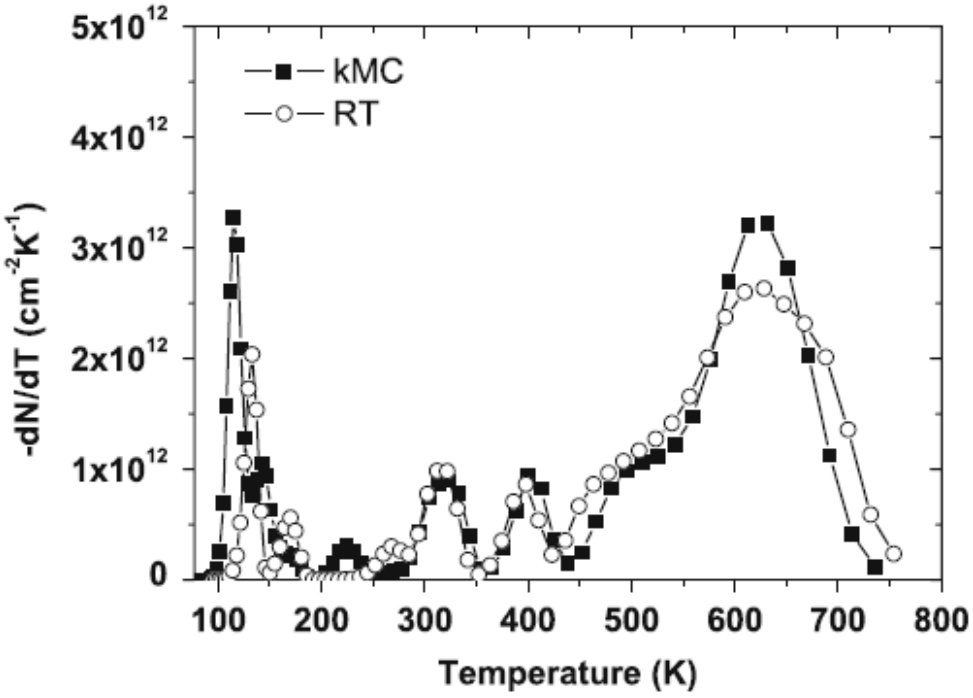
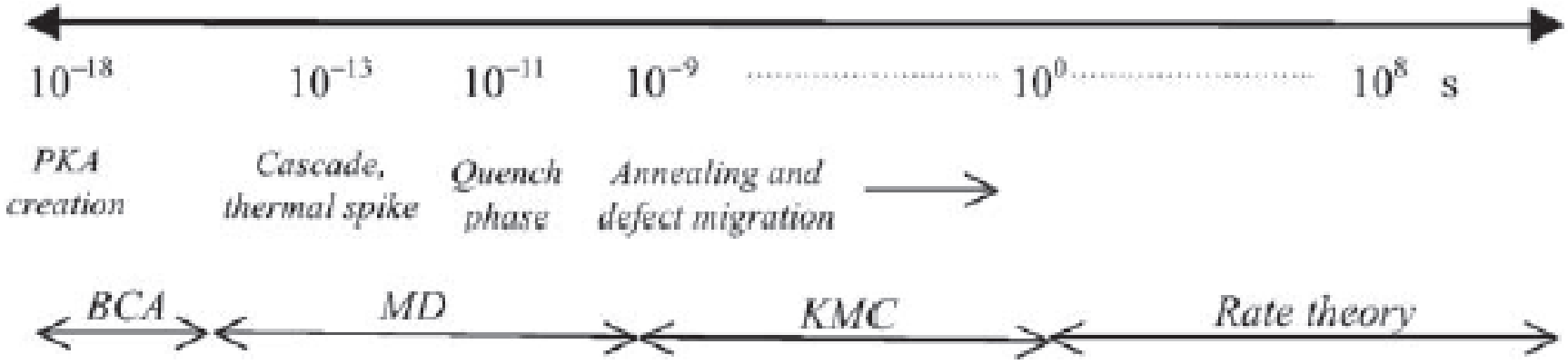


Fig. 2 Recovery stages predicted by kMC and RT models for a 30 keV Fe irradiation for a dose of 10^{-4} dpa

Damage Cascades – Summary

Was, p. 140

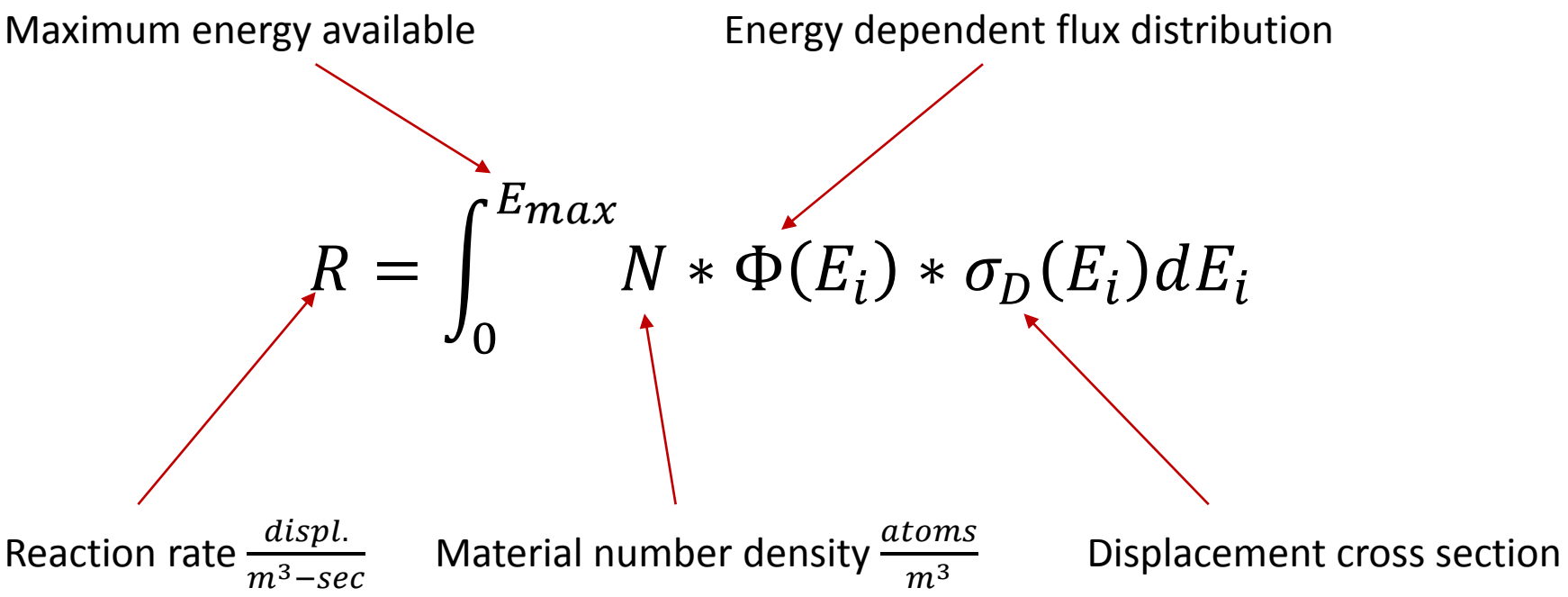
- Spans multiple time scales
  - Sets the stage for defect migration to higher length scales



  - Simulation also requires multiscale methods with much creativity to get right!

Displacement Theory

- Define a rate of atomic displacements using flux:



Displacement Theory

- Define a rate of atomic displacements using flux:

$$R = \int_0^{E_{max}} N * \Phi(E_i) * \sigma_D(E_i) dE_i$$

$$\frac{R}{N} = \frac{DPA}{sec} = \int_0^{E_{max}} \Phi(E_i) * \sigma_D(E_i) dE_i$$

Displacement Theory

- Define a rate of atomic displacements using flux:

$$\frac{DPA}{sec} = \int_0^{E_{max}} \Phi(E_i) * \sigma_D(E_i) dE_i$$

Known or pre-determined

Only unknown quantity

- Develop expression for displacement cross section

Displacement Theory

- Define a rate of atomic displacements using flux:

$$\frac{DPA}{sec} = \int_0^{E_{max}} \Phi(E_i) * \sigma_D(E_i) dE_i$$

Probability that an atom displaced by a particle with energy E_i leaves with recoil energy T (differential energy transfer cross section)

$$\sigma_D(E_i) = \int_{T_{min}}^{T_{max}} \sigma(E_i, T) v(T) dT$$

Number of atomic displacements from a PKA with energy T

- T is the PKA (displaced atom) recoil energy

Displacement Theory

$$\sigma_D(E_i) = \int_{T_{min}}^{T_{max}} \sigma(E_i, T)\nu(T)dT$$

- Assume there is some threshold energy (E_d) below which a displacement does not occur:

$$\nu(T) = 0; \quad T < E_d$$

- Otherwise a displacement will occur:

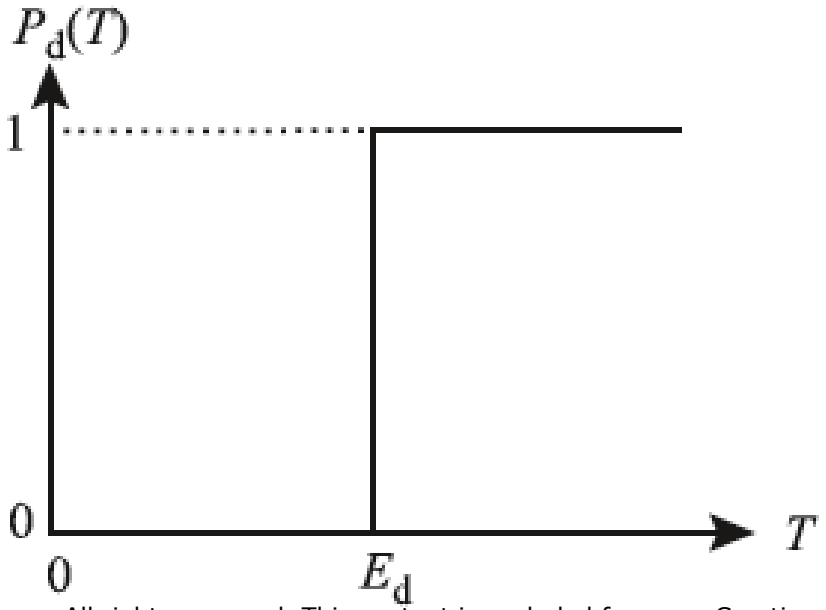
$$\nu(T) = 1; \quad T \geq E_d$$

Displacement Theory

Was, p. 74

$$\sigma_D(E_i) = \int_{T_{min}}^{T_{max}} \sigma(E_i, T)\nu(T)dT$$

- Sharp displacement threshold model:
- What does this model neglect?



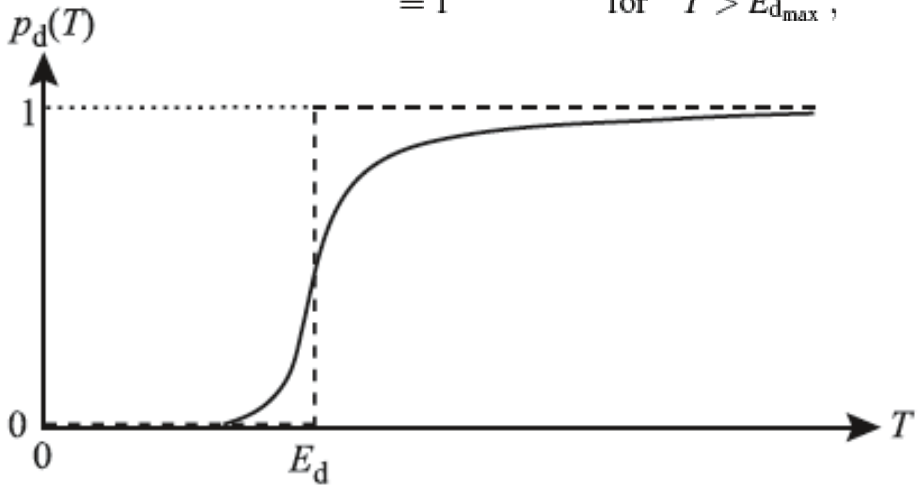
Displacement Theory

Was, p. 75

$$\sigma_D(E_i) = \int_{T_{min}}^{T_{max}} \sigma(E_i, T)\nu(T)dT$$

- Add some smoothness to this function:
- Accounts for atomic vibrations, impurities

$$\begin{aligned} P_d(T) &= 0 && \text{for} \quad T < E_{d_{min}} \\ &= f(T) && \text{for} \quad E_{d_{min}} < T < E_{d_{max}} \\ &= 1 && \text{for} \quad T > E_{d_{max}} \end{aligned},$$



Displacement Theory

- What is this threshold energy?
  - Let's estimate?

1. Energy to break metal surface bonds: ~5eV
2. Shift removed atom to the interior: x2
3. Stuff atom in an interstitial site, assume no time to relax the lattice: x2
4. Displacement isn't in the easiest direction: x2

Displacement Theory

Was, p. 83

- What is this threshold energy?
- Notice any patterns in the data?
  - Crystal structure?
  - Melting point?
  - Something else?

Metal	Lattice (c/a)	$E_{d,min}$ (eV)	E_d (eV)
Al	fcc	16	25
Ti	hcp (1.59)	19	30
V	bcc	–	40
Cr	bcc	28	40
Mn	bcc	–	40
Fe	bcc	20	40
Co	fcc	22	40
Ni	fcc	23	40
Cu	fcc	19	30
Zr	hcp	21	40
Nb	bcc	36	60
Mo	bcc	33	60
Ta	bcc	34	90
W	bcc	40	90
Pb	fcc	14	25
Stainless steel	fcc		40

Displacement Theory

$$\sigma_D(E_i) = \int_{T_{min}}^{T_{max}} \sigma(E_i, T) v(T) dT$$

- Returning to *v(T)*, assume sufficiently high energy PKAs can do more damage!
- Enter the *Kinchin-Pease* (K-P) model

Kinchin-Pease Model

$$v(T) = \frac{2}{T}\left[\int_0^T v(\varepsilon)d\varepsilon\right]$$

- Now split into three relevant ranges:

$$\mathrm{E} < E_d, \qquad E_d \leq \mathrm{E} < 2E_d, \qquad \mathrm{E} > 2E_d$$

$$v(T) = \frac{2}{T}\left[\int_0^{E_d} v(\varepsilon)d\varepsilon + \int_{E_d}^{2E_d} v(\varepsilon)d\varepsilon + \int_{2E_d}^{T} v(\varepsilon)d\varepsilon\right]$$

Kinchin-Pease Model

$$\nu(T) = \frac{2}{T}\left[\int_0^{E_d} \nu(\varepsilon)d\varepsilon + \int_{E_d}^{2E_d} \nu(\varepsilon)d\varepsilon + \int_{2E_d}^{T} \nu(\varepsilon)d\varepsilon\right]$$

- First term is **0** (energy too low to displace)
- Second term is **1** (only one displacement possible)
- Third term is steadily increasing

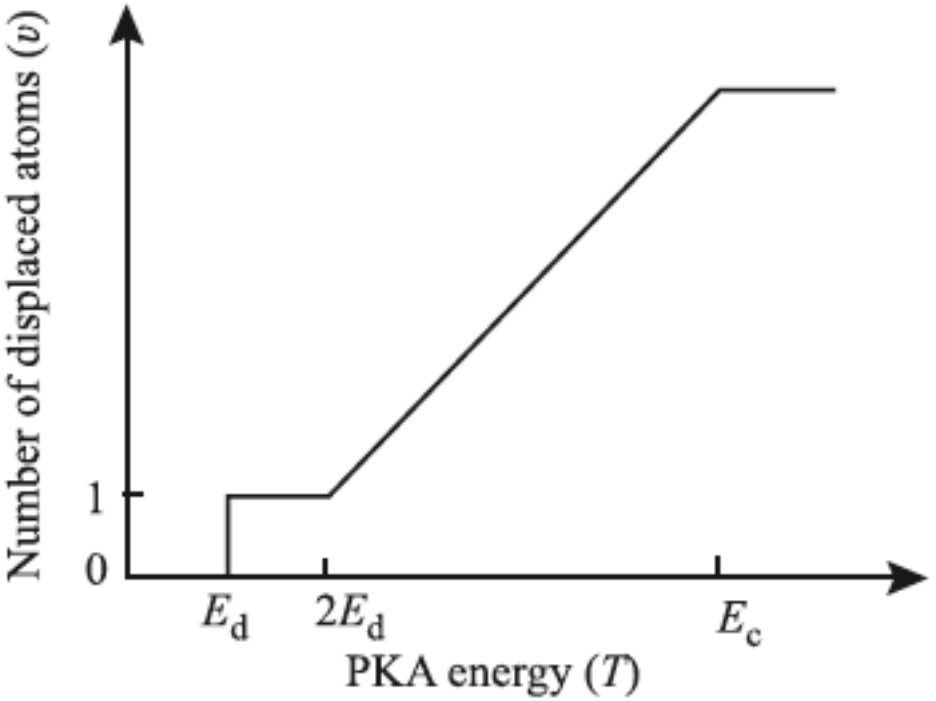
$$\nu(T) = \frac{2}{T}\left[\int_0^{E_d} 0d\varepsilon + \int_{E_d}^{2E_d} 1d\varepsilon + \int_{2E_d}^{T} \nu(\varepsilon)d\varepsilon\right]$$

Kinchin-Pease Model

Was, p. 77

- Final formulation:

$$\nu(T) = \begin{cases} 0 & \text{for } T < E_d \\ 1 & \text{for } E_d < T < 2E_d \\ \dfrac{T}{2E_d} & \text{for } 2E_d < T < E_c \\ \dfrac{E_c}{2E_d} & \text{for } T \geq E_c \end{cases}$$

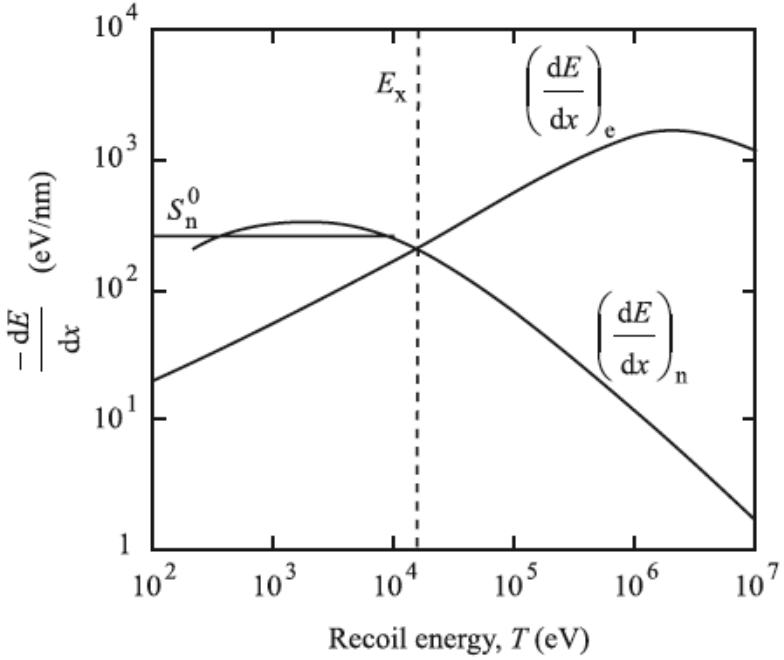


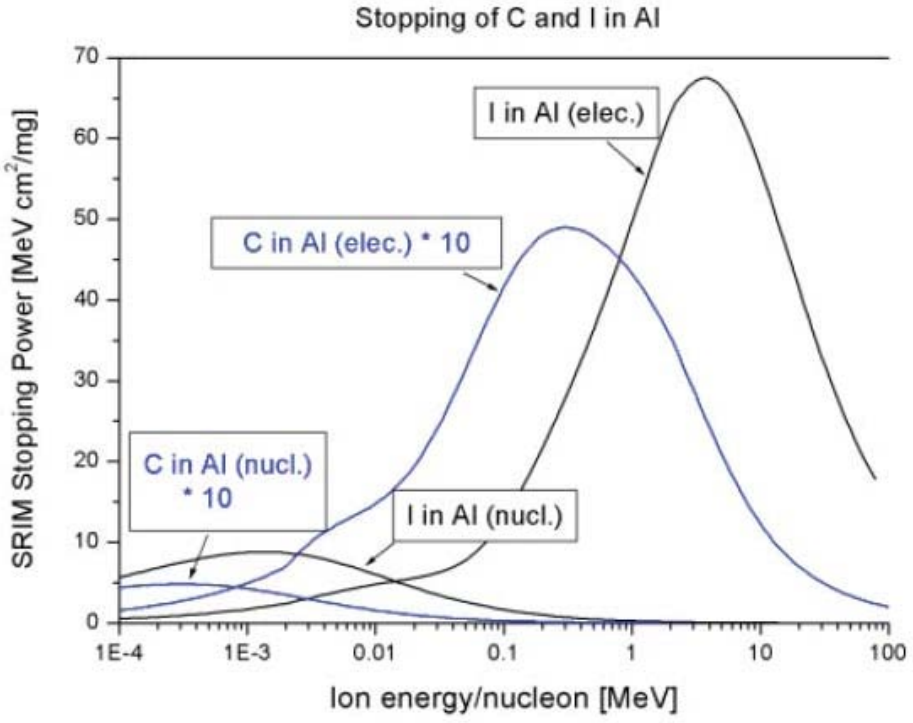
Modifications to K-P Model

Was, p. 84

H. Paul. *AIP Conf. Proc.* 1525:309 (2013)

- Is the cutoff energy really true?

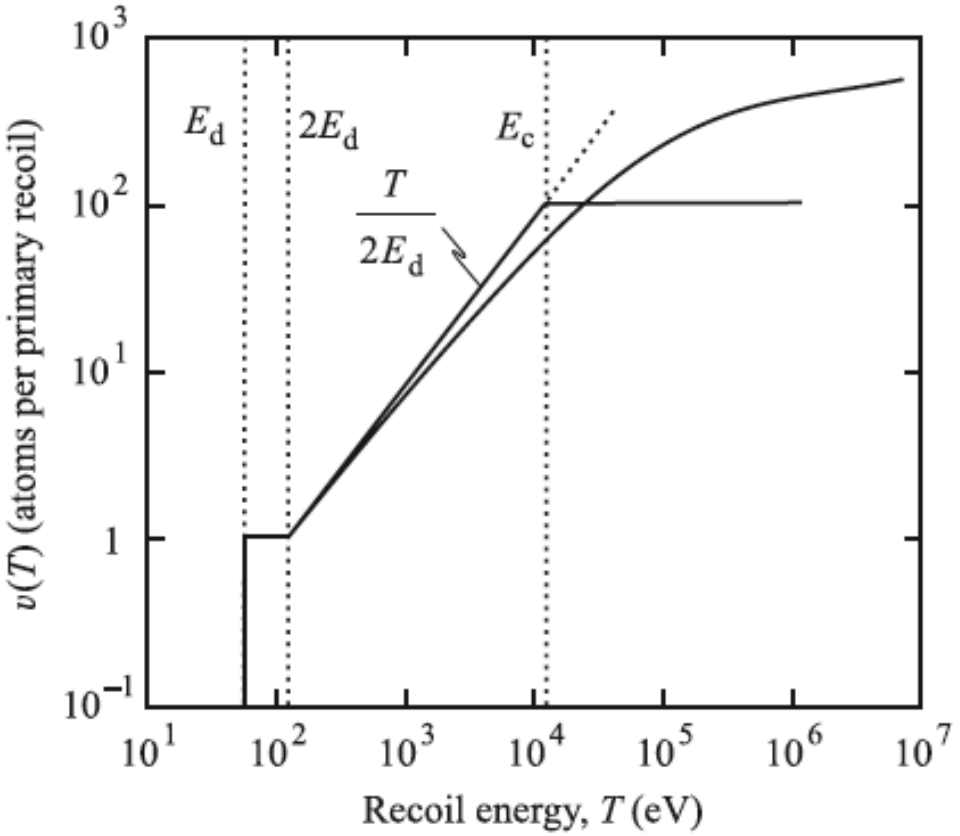




Modifications to K-P Model

Was, p. 77

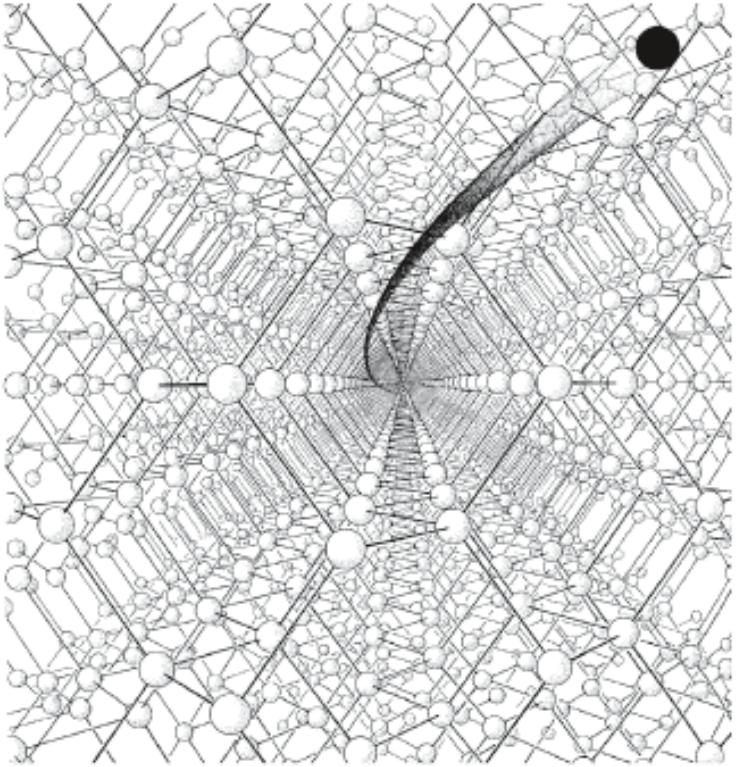
- Allow nuclear stopping power to diminish, but not disappear, after E_c
- Also allow electronic stopping to start taking over before E_c



Modifications to K-P Model

Was, p. 102

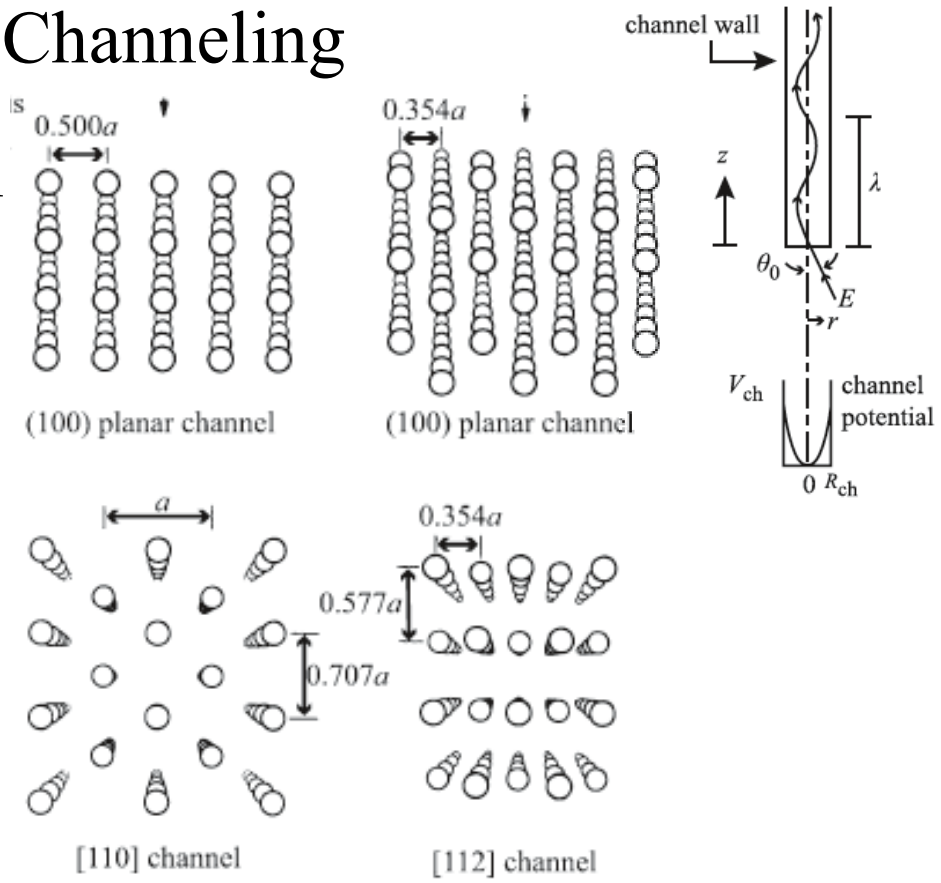
- Account for crystallinity: Channeling
- Displaced atom can travel through empty space between lattice planes
  - Nuclear stopping ~ 0
  - Only electronic stopping



Modifications to K-P Model

Was, p. 102

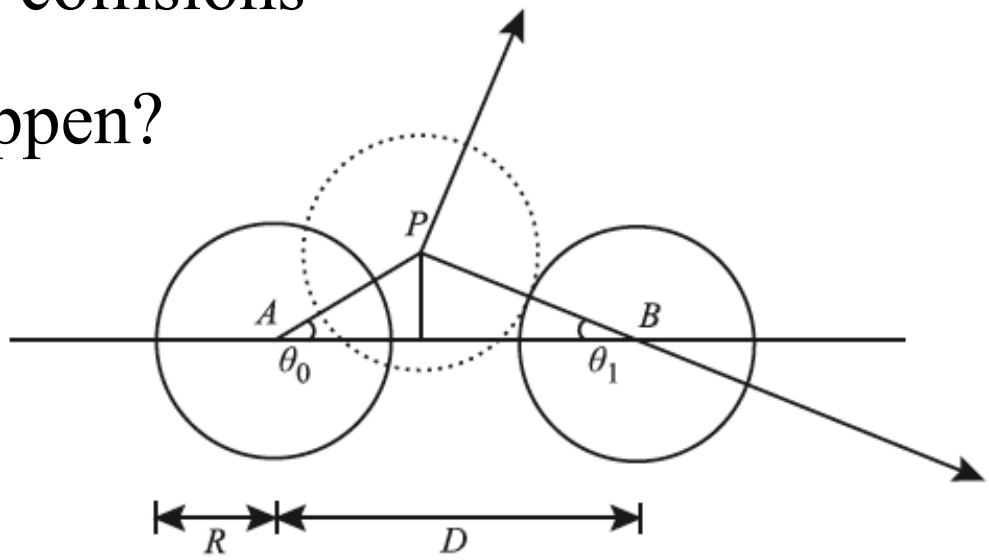
- Account for crystallinity: Channeling
- Displaced atom can travel through empty space between lattice planes
  - Nuclear stopping ~ 0
  - Only electronic stopping
- Lots of paths to channel!



Modifications to K-P Model

Was, p. 92

- Close-packed energy transfer: Focusing
  - Think packed billiard balls on a pool table
- Assumes hard sphere collisions
- Where would this happen?
  - Close-packed directions
  - Crowdions
  - Dumbbells



The Real σ_D Is Ugly!

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Damage After the Cascade

- What happens to damage after the cascade?
  - Production
  - Recombination
  - Absorption at sinks
  - Migration

Point Defect Balance

Change = Gain – Loss

- What are the possible gain terms?
  - Displacement production
  - Reaction production
- What are the possible loss terms?
  - Recombination
  - Loss to sinks
  - Diffusion

Point Defect Balance

Change = Gain – Loss

- What are the possible sinks?
  - Grain boundaries
  - Dislocations
  - Impurities
  - Free surfaces
  - Incoherent precipitates

Gain Terms

- Defect Production Rate:

From SRIM, etc.

$$K_0 = \left(\frac{DPA}{sec}\right) * \varepsilon$$

Damage cascade efficiency

- Reaction Production Rate:

Ignore… for now

$$R_0 = \sum_{d=1}^{n} Rxn_d$$

Loss Terms: Recombination

- Introduce some recombination rate constant: K_{iv}
- Relate to the relevant defect concentrations:

$$C_i = Interstitial\ Concentration$$

$$C_v = Vacancy\ Concentration$$

$$\left.\frac{\partial C_{(i,v)}}{\partial t}\right|_{Recombination} = K_{iv} C_i C_v$$

Loss Terms: Sinks

- For each sink, define a sink strength: K_s
- Relate sink rate to concentrations of defects $C_{(i,v)}$ and sinks:

$$\left.\frac{\partial C_{(i,v)}}{\partial t}\right|_{Sinks} = -\sum_{s=1}^{All\ Sinks} K_s C_{(i,v)} C_s$$

Loss Terms: Diffusion

- We already know this equation from Fick's Law:

$$\left.\frac{\partial C_{(i,v)}}{\partial t}\right|_{Diffusion} = \nabla D_{(i,v)} \nabla C_{(i,v)}$$

Combining Terms:

$$\frac{\partial C_{(i,v)}}{\partial t} = \left(\frac{DPA}{sec}\right) * \varepsilon - K_{iv} C_i C_v - \sum_{s=1}^{All\ Sinks} K_s C_{(i,v)} C_s + \nabla D_{(i,v)} \nabla C_{(i,v)}$$

Neglect Spatial Variance:

$$\frac{\partial C_i}{\partial t} = K_0 - K_{iv} C_i C_v - \sum_{s=1}^{All\ Sinks} K_s C_i C_s$$

$$\frac{\partial C_i}{\partial t} = K_0 - K_{iv} C_i C_v - \sum_{s=1}^{All\ Sinks} K_s C_v C_s$$

Note on Vacancy Conc.

- C_v must be adjusted to account for thermal vacancies:

$$C_v^* = C_v - C_v^0$$

Adjusted vacancy concentration

Total vacancy concentration

Thermal vacancy concentration

- Why do we ignore this for interstitials?
  - Equilibrium interstitial concentration is so low!

Equilibrium Defect Conc.

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Limiting Cases of Point Defect Kinetic Equations

- (1) Assume low temperature, low sink densities

$$\frac{\partial C_v}{\partial t} = K_0 - K_{iv} C_i C_v - \sum_{s=1}^{All\ Sinks} K_s C_v C_s + \nabla D_v \nabla C_v$$

$$\frac{\partial C_i}{\partial t} = K_0 - K_{iv} C_i C_v - \sum_{s=1}^{All\ Sinks} K_s C_i C_s + \nabla D_i \nabla C_i$$

Case 1: Low T, Low C_s

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Case 1: Low T, Low C_s

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Case 1: Low T, Low C_s

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What's In a Sink Term?

$$K_{iv} = 4\pi r_{iv}(D_i + D_v)$$

Sink Strength

Interaction radius

Diffusivities

$$K_{is} = 4\pi r_{is}(D_i)$$

$$K_{vs} = 4\pi r_{vs}(D_v)$$

Case 2: Low T, Medium C_s

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Case 2: Low T, Medium C_s

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Case 2: Low T, Medium C_s

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Case 2: Low T, Medium C_s

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Compare Cases 1 & 2

Was, pp. 194, 197

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Case 3: Low T, High C_s

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Case 3: Low T, High C_s

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Case 3: Low T, High C_s

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Case 3: Low T, High C_s

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Case 3: Low T, High C_s

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Compare Cases 2 & 3

Was, pp. 197, 198

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Case 4: High Temperature

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Case 4: High Temperature

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Case 4: High Temperature

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Case 4: High Temperature

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Compare Cases 3 & 4

Was, pp. 198, 200

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Where Does This Model Break Down?

- Near sinks
- Sinks with biases for defects
  - Interaction radii
  - Defect-dependent sinks
- Time-variant sinks
- Time-variant anything else
- *Spatial variance*

Return Spatial Variance

$$\frac{\partial C_v}{\partial t} = K_0 - K_{iv} C_i C_v - \sum_{s=1}^{Sinks} K_s C_v C_s + \nabla D_v \nabla C_v$$

$$\frac{\partial C_i}{\partial t} = K_0 - K_{iv} C_i C_v - \sum_{s=1}^{Sinks} K_s C_i C_s + \nabla D_i \nabla C_i$$

- What's in a *D* anyway?

Radiation Enhanced Diffusion

- D_a (diffusivity of a type of atom) is a sum of all relevant effects
  - Some are turned on by radiation (interstitialcy)
  - Some are enhanced by radiation (vacancy)

$$D_a = \sum_{d=1}^{Defects} f_d D_a^d C_d$$

$$D_a = f_V D_a^v C_v + f_i D_a^i C_i + f_{2v} D_a^{2v} C_{2v} + f_{crowdion} D_a^{crowdion} C_{crowdion} + f_{dumbbell}\, D_a^{dumbbell} C_{dumbbell} \cdots$$

Components of Radiation Enhanced Diffusion

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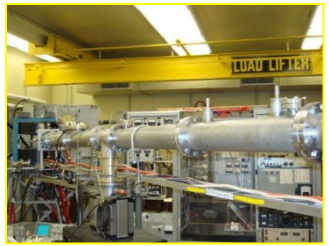
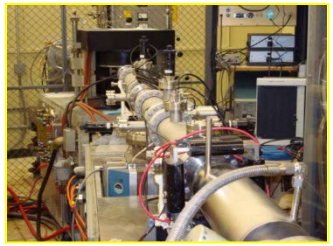
Returning Spatial Dependence: Case Study

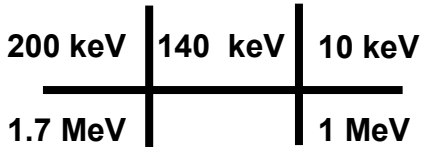
- 1D ion irradiation, includes:
  - A free surface
  - Dislocations
  - Thermal vacancies (not interstitials)
  - Differing interaction radii
  - Spatially dependent defect production
  - Injected interstitials

Experimental Evidence

- 99.995% Fe
  - 3.5MeV Fe^{+2} self-ions, 450C, ~1mA beam current
    - $1.8 \cdot 10^{-3}$ dpa/s
  - Peak doses:
    - 35, 75, 105dpa
  - Characterization:
    - TEM
    - Image analysis



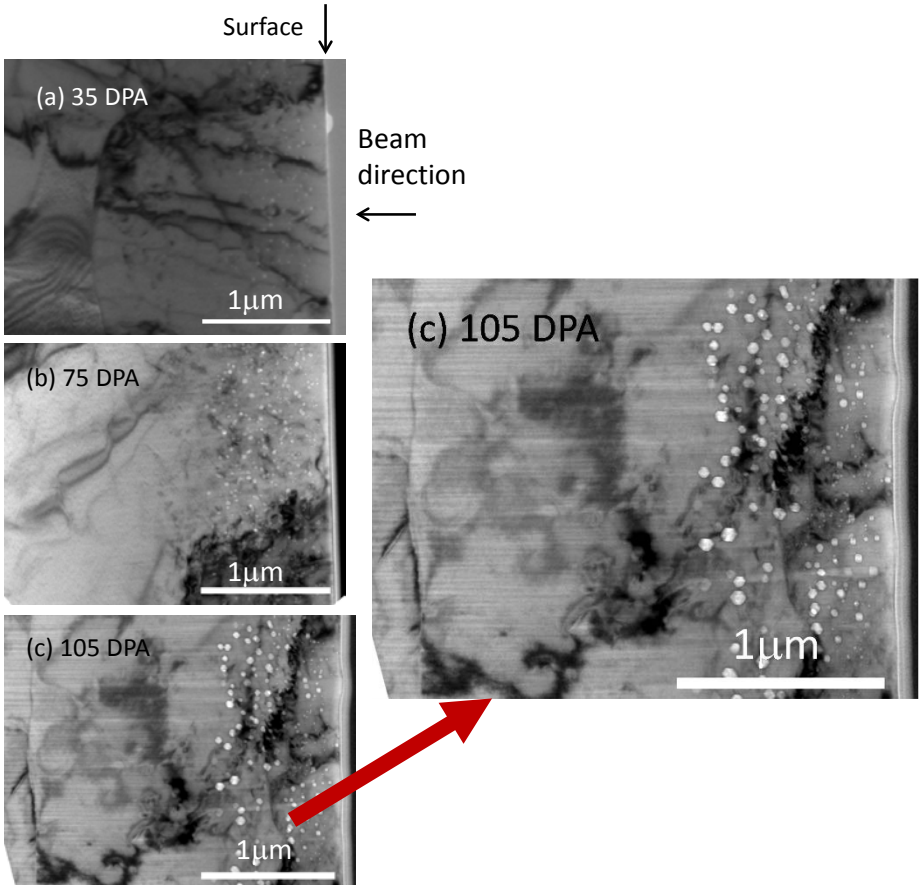


Courtesy of Lin Shao. Used with permission.

Experimental Evidence

- Void swelling is observed below material surface
  - No swelling observed beyond 1μm depth
  - Range of Fe^{+2} ions is ~1.5μm

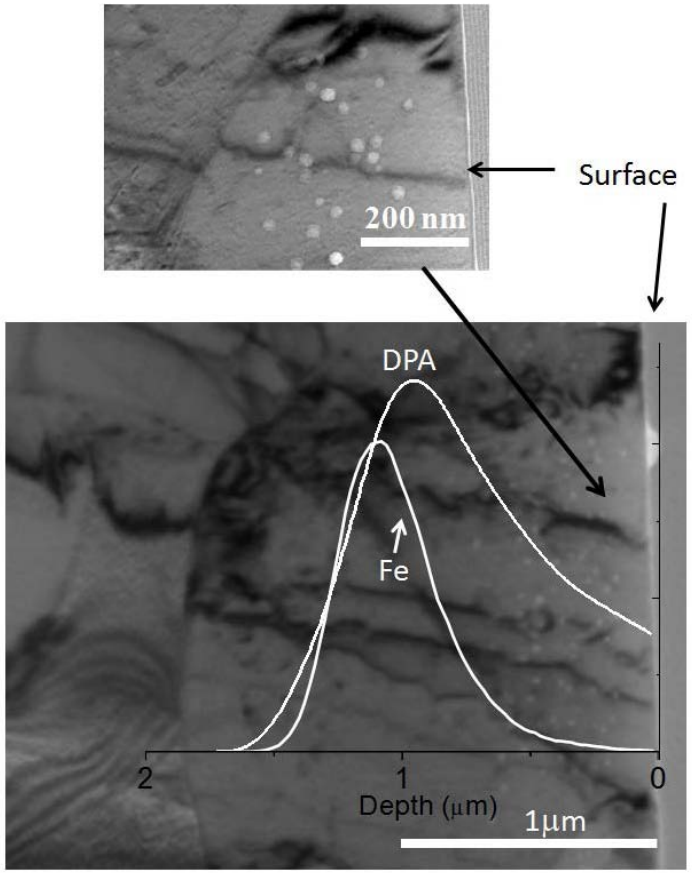


L. Shao et al. (2014)

Courtesy of Lin Shao. Used with permission.

Experimental Evidence

- Correlate damage (point defect creation) with injected interstitials

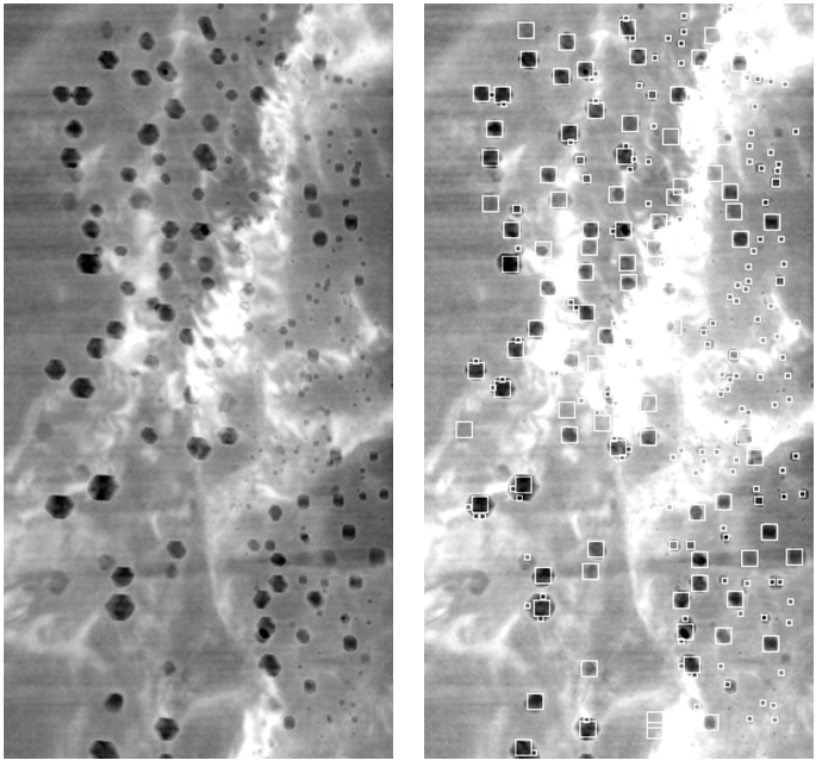


L. Shao et al. (2014)

Courtesy of Lin Shao. Used with permission.

Experimental Evidence

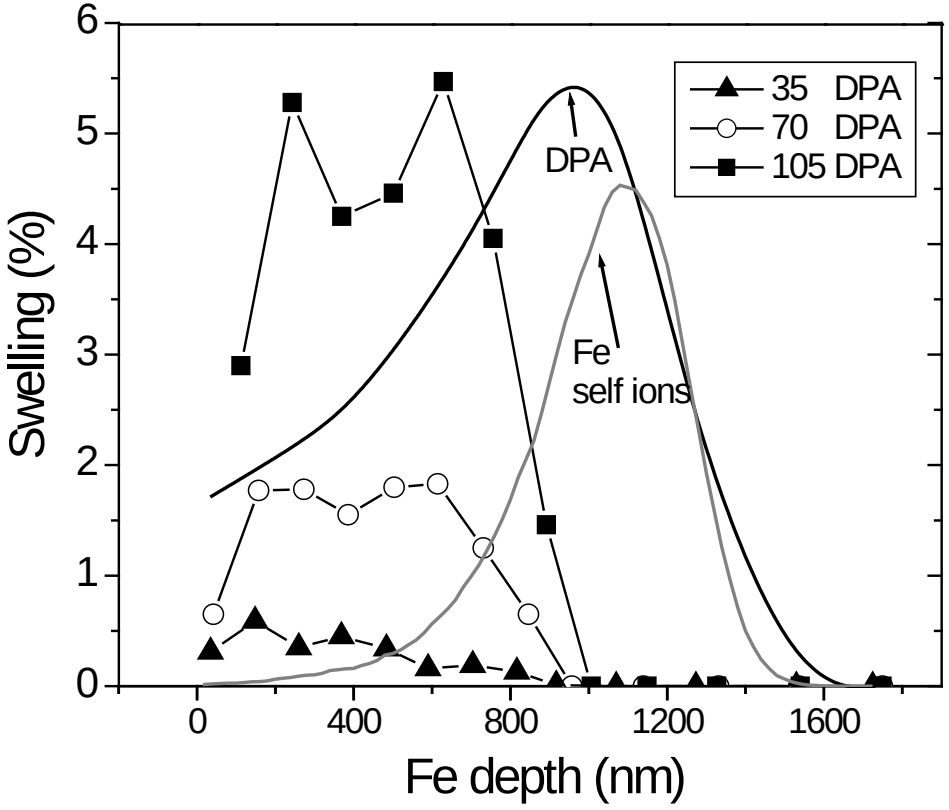
- Image analysis used to estimate void fraction vs. distance
  - Squares identify voids



L. Shao et al. (2014)

Experimental Evidence

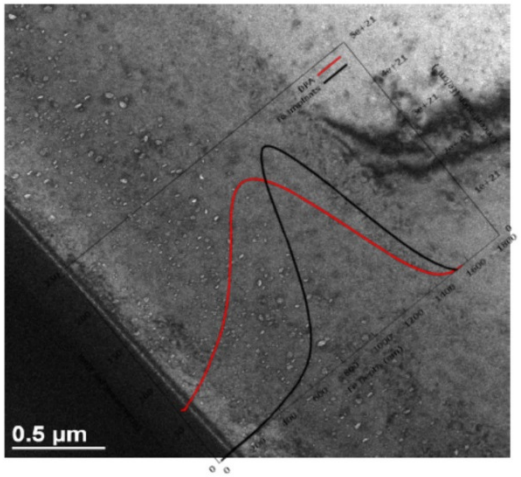
- Correlate damage (point defect creation) with injected interstitials
  - Voids not observed near injected interstitials



L. Shao et al. (2014)

More Experimental Evidence

- Occurs in complex alloys as well
- This is a highly general phenomenon!



MA956 ODS alloy

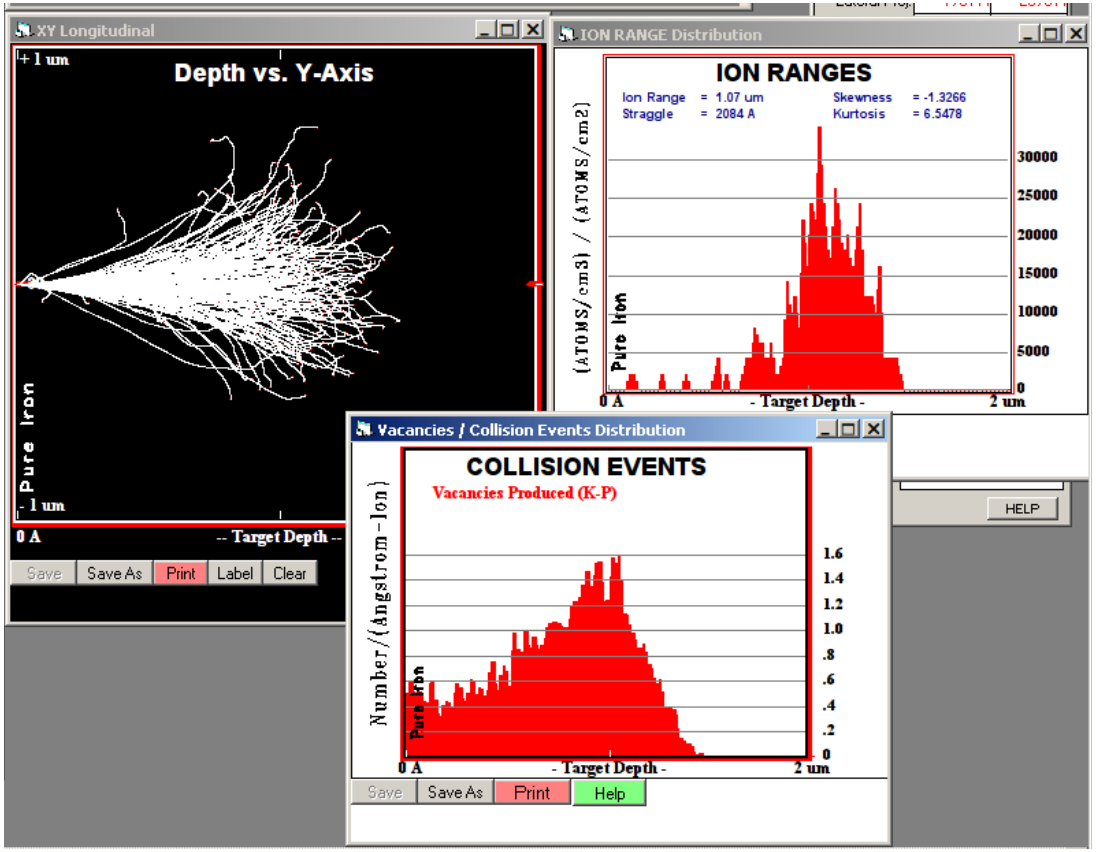
3.5 MeV F^{e+} at 425°C

200 dpa at peak damage position

F. A. Garner, M. B. Toloczko, A. Certain, L. Shao, J. Gigax, C. Wei, "Impact of the Injected Interstitial Effect on Ion-Induced Void Swelling in Austenitic and Ferritic-ODS Alloys," TMS Poster (2014)

Modeling & Simulation Explains the Mechanism

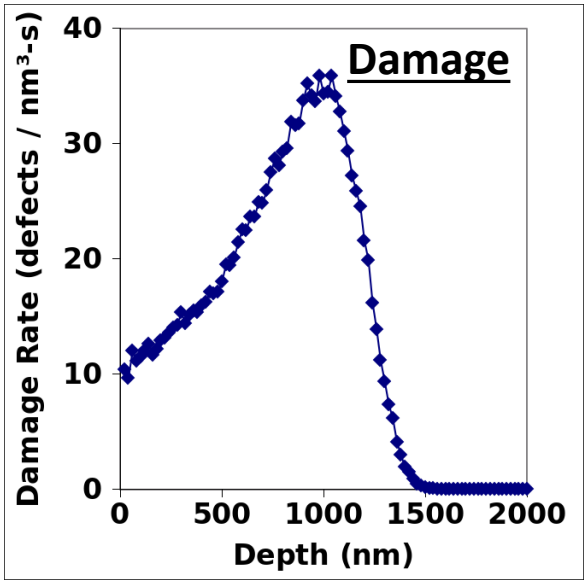
- Used SRIM* computer code to calculate damage rate (dpa/s) and implantation rate (Fe/cm^3-s)

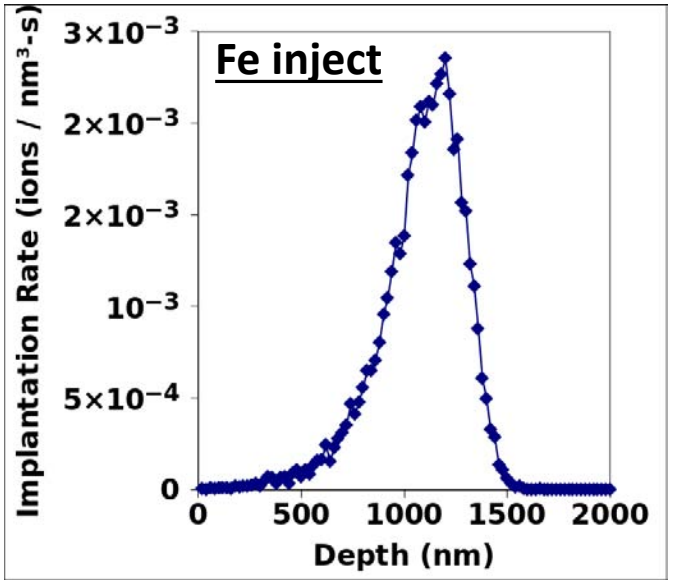


*Stopping Range of Ions in Matter

Modeling & Simulation Explains the Mechanism

- Simultaneously plot damage (V + I) and injected interstitials (I only)





Modeling & Simulation Explains the Mechanism

- Use SRIM data as forcing function for point defect balance equations
- Assumptions:
  - $E_M^I = 0.18eV$ (<110> split dumbbell is dominant interstitial defect)
  - $E_M^V = 0.66eV$ (atomically pure iron) or 1.1eV (realistic purity)
  - Neglect formation of larger vacancy or interstitial defects
  - Defects can annihilate by diffusion, network dislocations, incoherent precipitates, nucleated voids, recombination, free surface annihilation

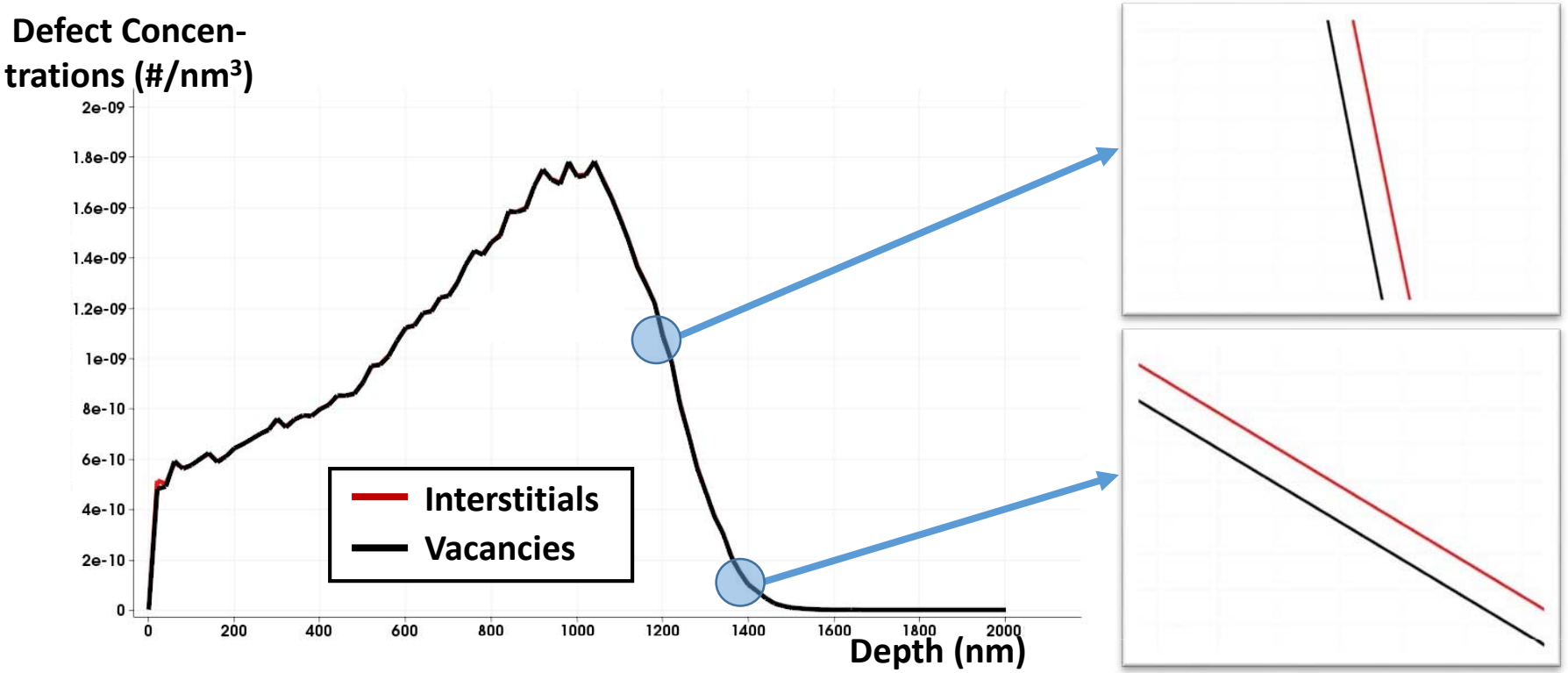
Simulation Framework

- MOOSE – Multiphysics Object Oriented Simulation Environment
  - Greatly simplifies creating simulations quickly
  - Seamless ability to fully couple ODEs & PDEs on a finite element framework
  - **Recently open sourced:** ***www.mooseframework.com***

ODE – Ordinary differential equation
PDE – Partial differential equation

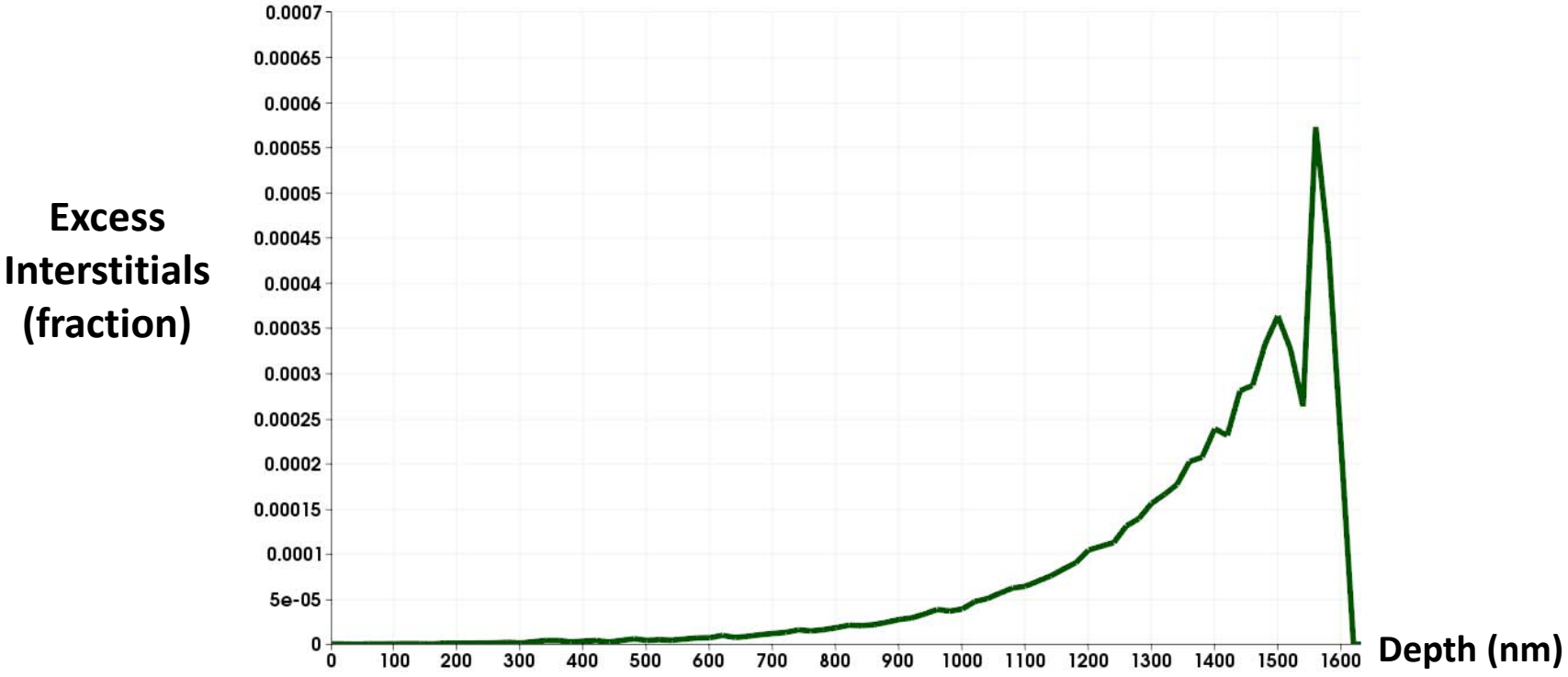
Modeling & Simulation Explains the Mechanism

- Superimpose both point defect plots



Modeling & Simulation Explains the Mechanism

- Plot *excess interstitial fraction*



Quantifying the Injected Interstitial Effect

- *Artificially* "turn off" injected interstitials
- Run side-by-side simulations, all other parameters equal

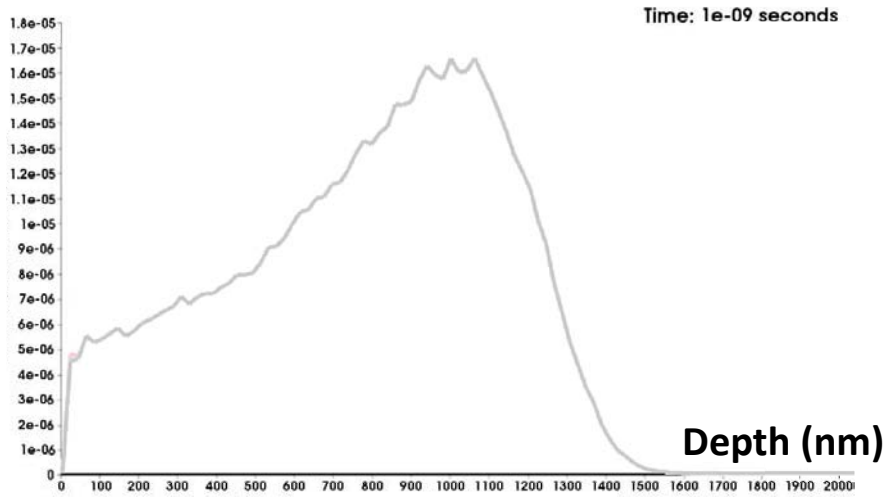
```
[hereiam][~/projects/trunk/grime]> diff grime.i grime-noII.i
193d192
<     SecondarySource = InjectedInterstitials
495c494
<   file_base = grime
---
>   file_base = grime-noII
[hereiam][~/projects/trunk/grime]>
```

Screenshot showing difference in input files

Results – Point Defects

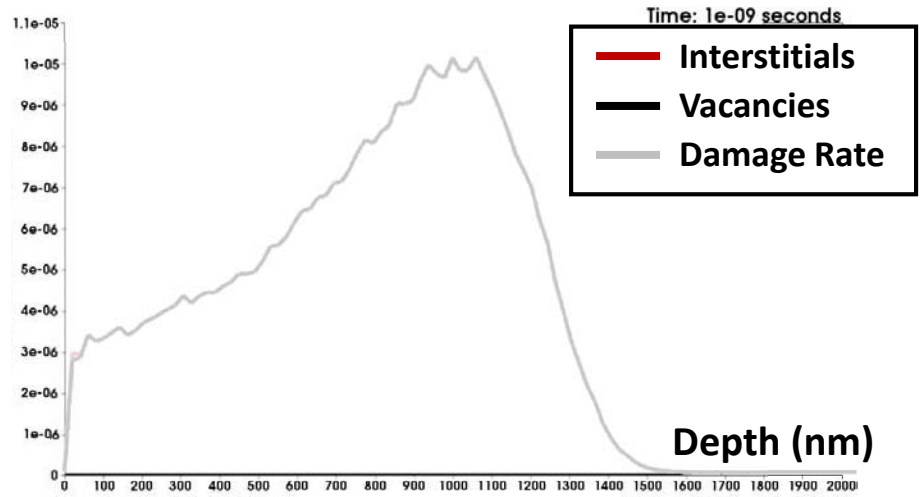
3.5MeV Fe^{+2}, 1mA, $1mm^2$ beam, 450C, E_M^V = 0.66eV

Point defects follow SRIM forcing function



Without **injected interstitials**

Point defects do not quite follow SRIM forcing function

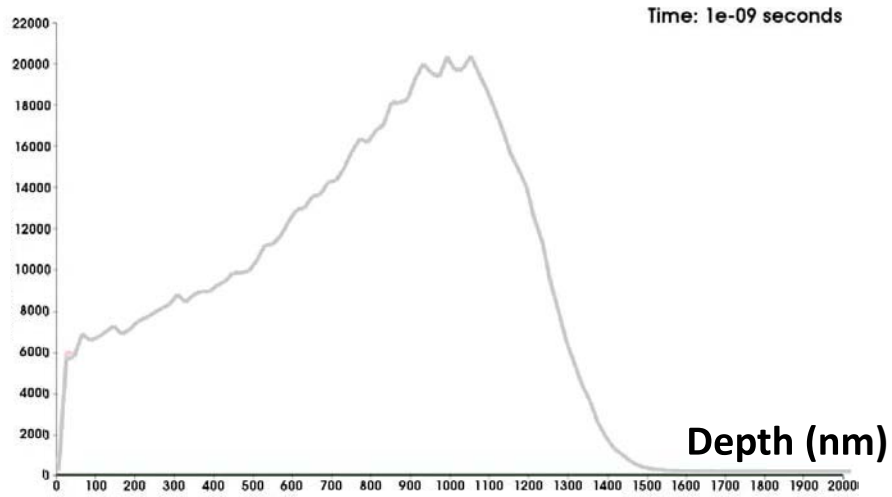


With **injected interstitials**

Results – Vacancy Supersaturation

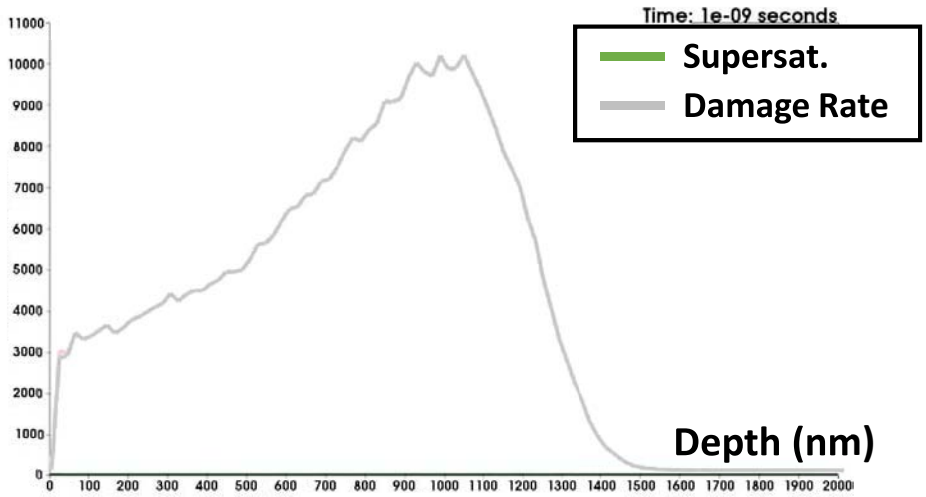
3.5MeV Fe^{+2}, 1mA, $1mm^2$ beam, 450C, E_M^V = 0.66eV

Peaks near maximum damage region



Without **injected interstitials**

Bimodal distribution, shifted to the left by 100nm

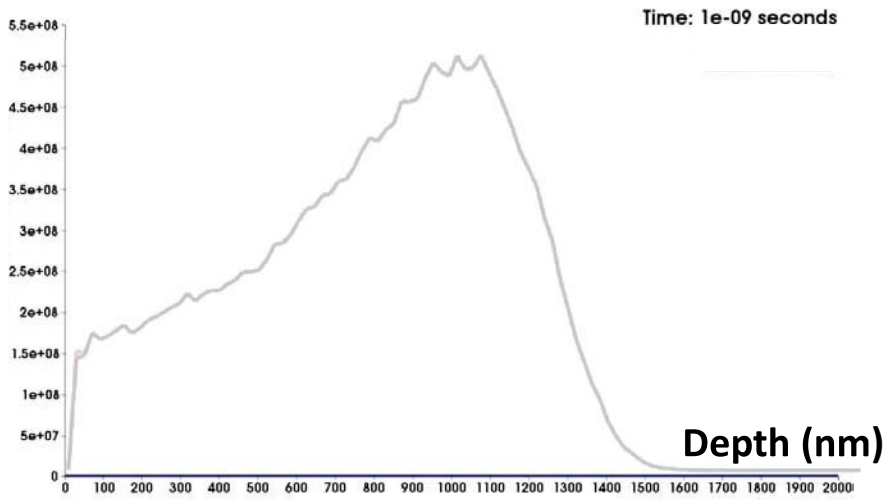


With **injected interstitials**

Results – Void Nucleation Rate

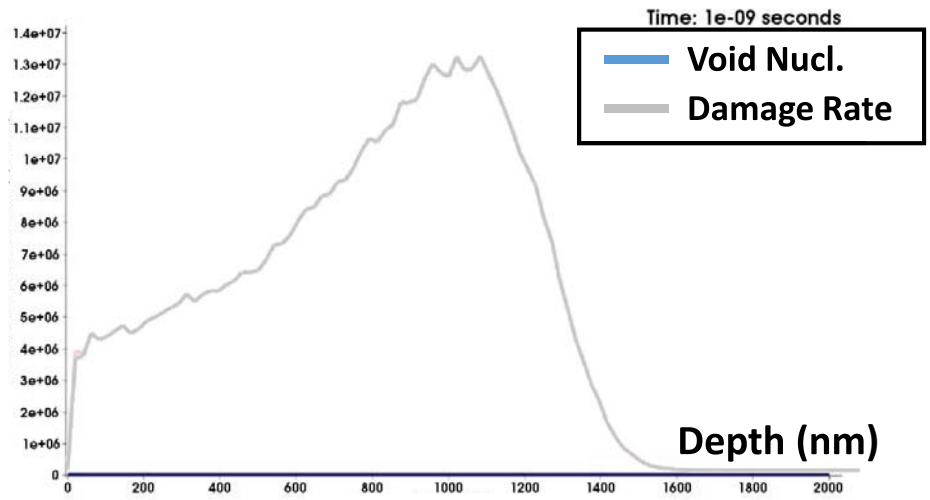
3.5MeV Fe^{+2}, 1mA, $1mm^2$ beam, 450C, E_M^V = 0.66eV

Clearly peaks at maximum damage region



Without **injected interstitials**

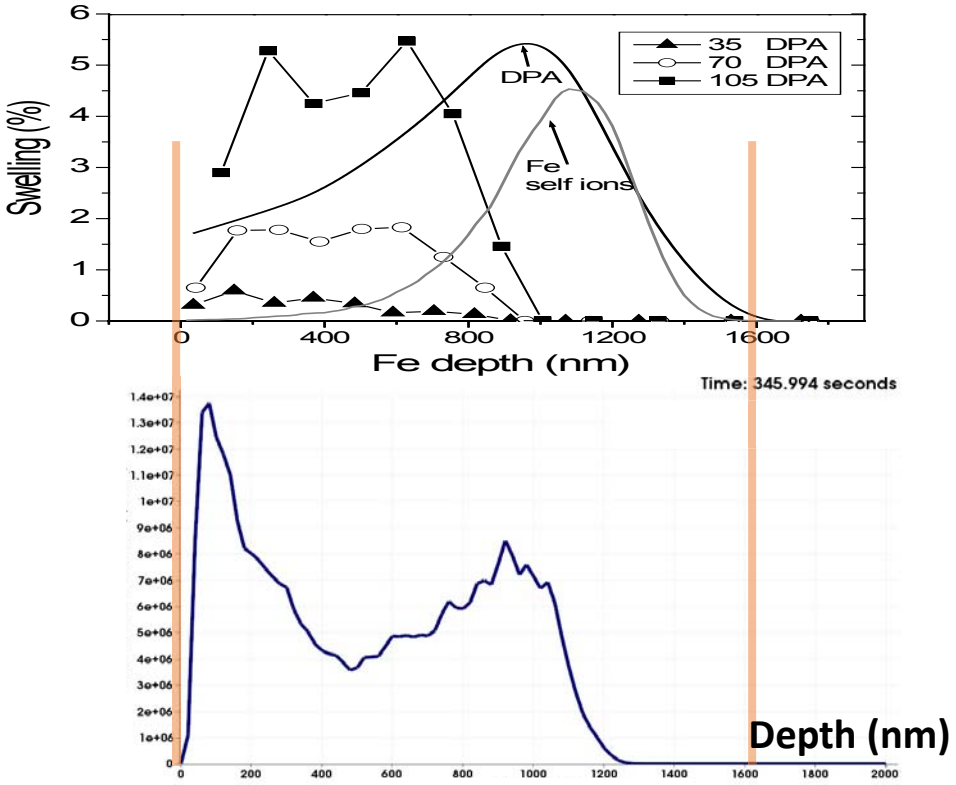
Very bimodal distribution, shifted to the left by 100nm



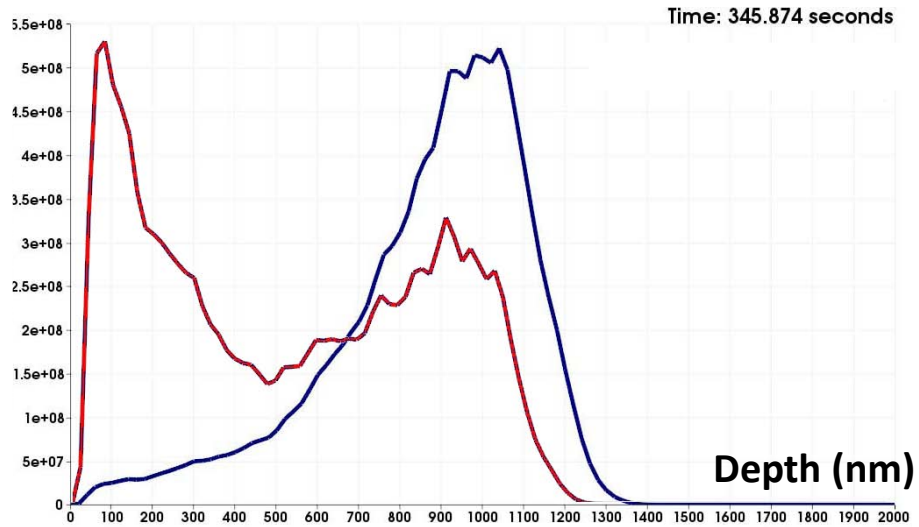
With **injected interstitials**

Compare with Experiments

3.5MeV Fe^{+2}, 1mA, $1mm^2$ beam, 450C, E_M^V = 0.66eV



Simulation vs. Experiments



With / Without Injected Interstitials

Explanation

- Small spatial defect imbalance has large change in vacancy supersaturation at peak injected interstitial locations

- ***This in turn affects void nucleation rate***

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Spring 2015