Range and Cascades

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Modifications to K-P Model

3. Effect of crystallinity:

Focusing

Channeling

NRT Model

- NRT:

Accounts for Frenkel pair defect efficiency

Used in ASTM E693 to convert neutron flux to dose rate (dpa/s) for steels!!!

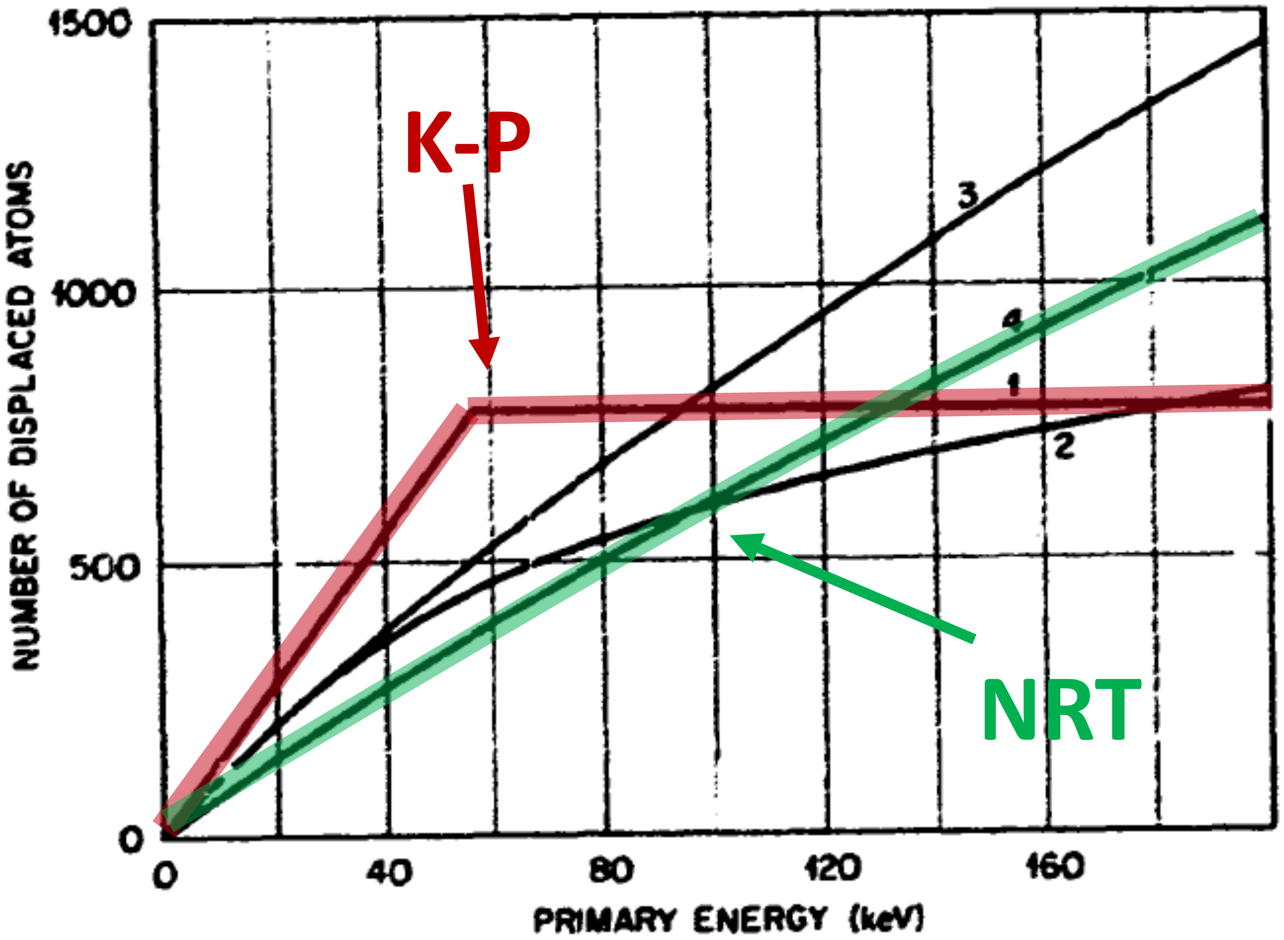

Fig. 2. Comparison of number of displaced atoms generated in bcc iron by a primary knock-on atom. Calculated results correspond to: (1) Kinchin–Pease model with $E_d = 40$ eV and $E_1 = 56$ keV; (2) the half-Nelson formula [4]; (3) earlier computer calculations of Norgett [18], using Torrens–Robinson computer simulation program [11]; and (4) the proposed formula, eqs (5)–(10).

A simple picture of slowing down

- The slowing down process of an ion impacting on a surface:

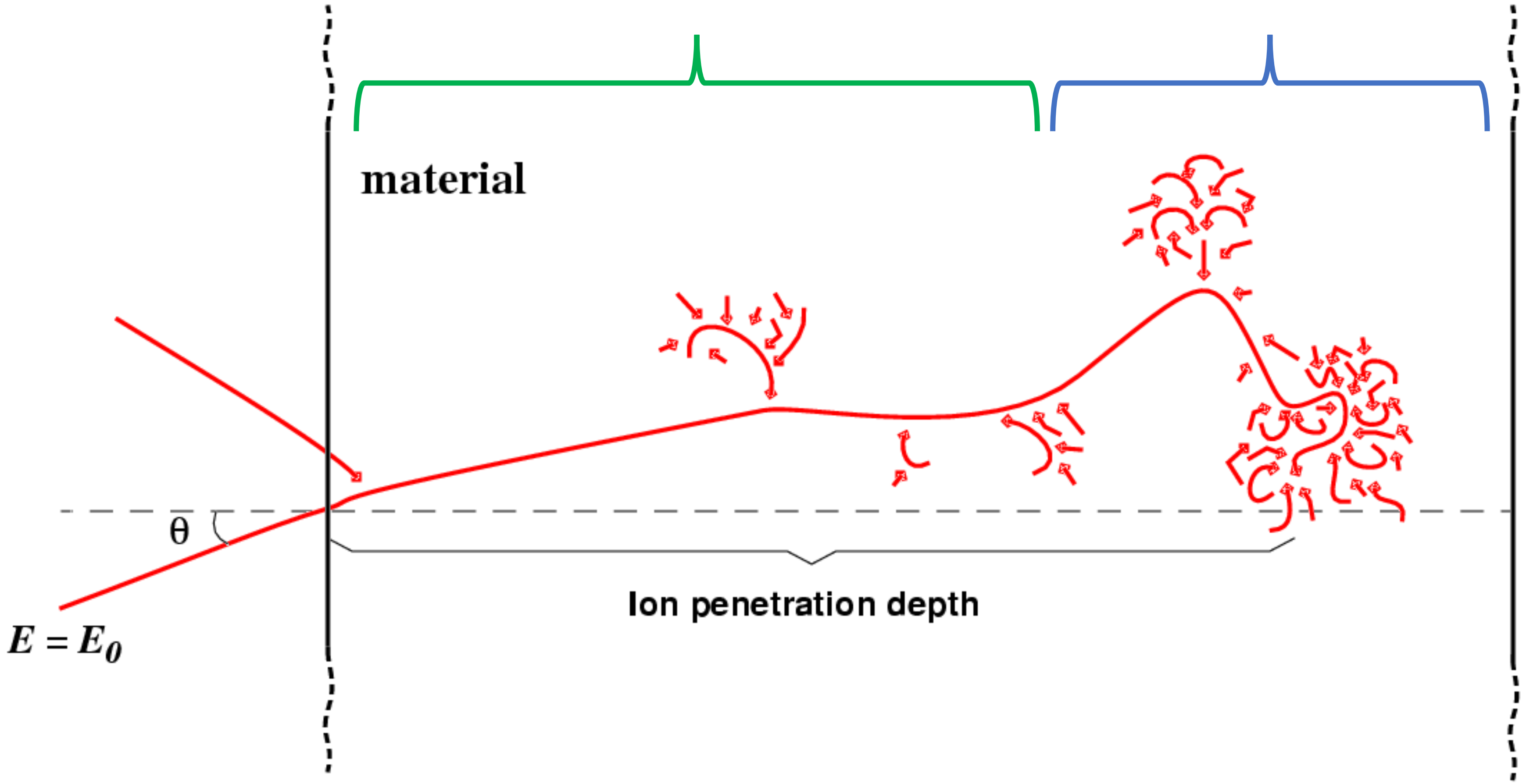

Image: Kai Nordlud

Outline

- Particle Distribution (**Range**):
  - Definition
  - Project Range
  - Standard Deviation
  - Concentration

- Goal: Calculate the **range** and **concentration** of implanted ions

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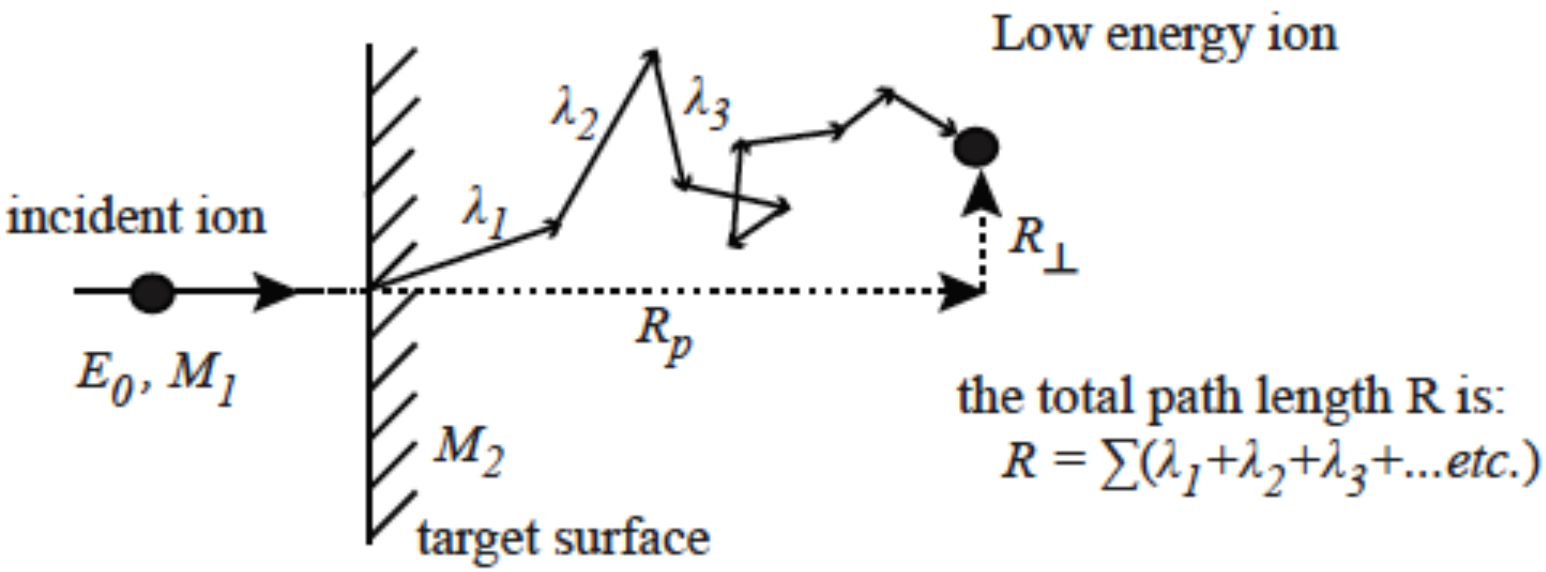
Definition of Range

- Range, R – total path travelled by a particle before it stops
- Projected Range, R_p – protection of R onto the initial direction of the projectile path



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Range

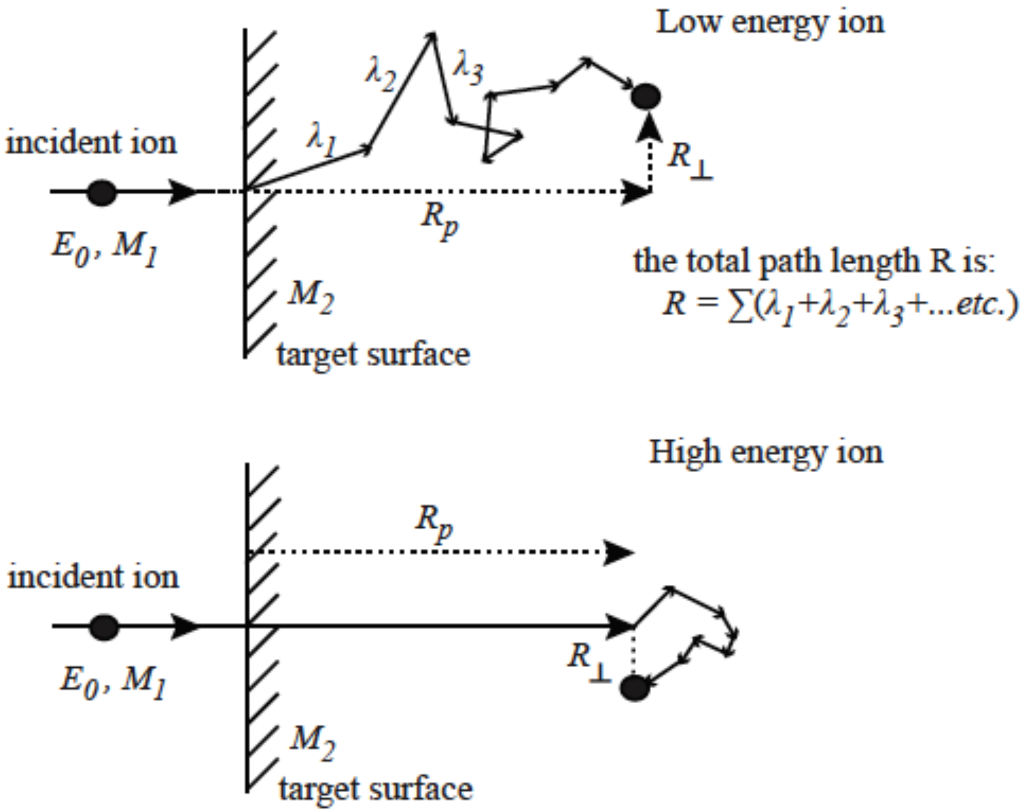
- Assume: Nuclear and electronic energy losses are independent:

$$S_T = S_n + S_e = \frac{1}{N}\left(\left(-\frac{dE}{d}\right)_n + \left(-\frac{dE}{dx}\right)_e\right)$$

- Integrate inverse of stopping power over the energy range of the particle:

$$Range = R = \int_0^{E_{max}} \frac{1}{S(E)}\,dE$$

$$R = \int_0^{E_{max}} \frac{dE}{S_n(E) + S_e(E)}$$



Simple Example

- Protons by electronic energy loss

Example

- Determine the range using the appropriate potential considering $E_i < E_{C}$:

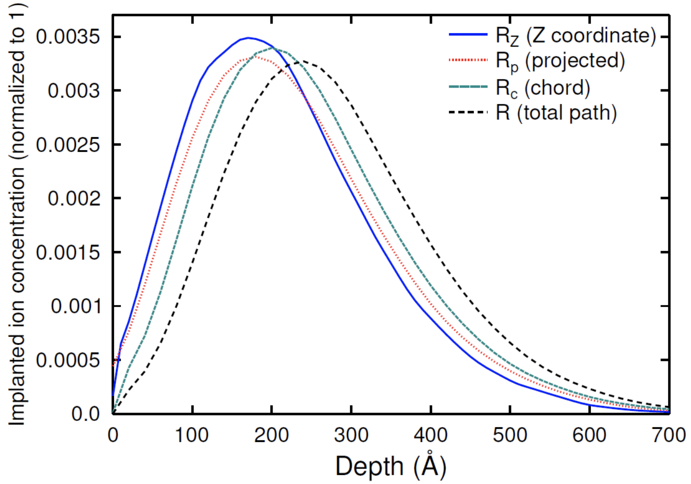
Modifications for range

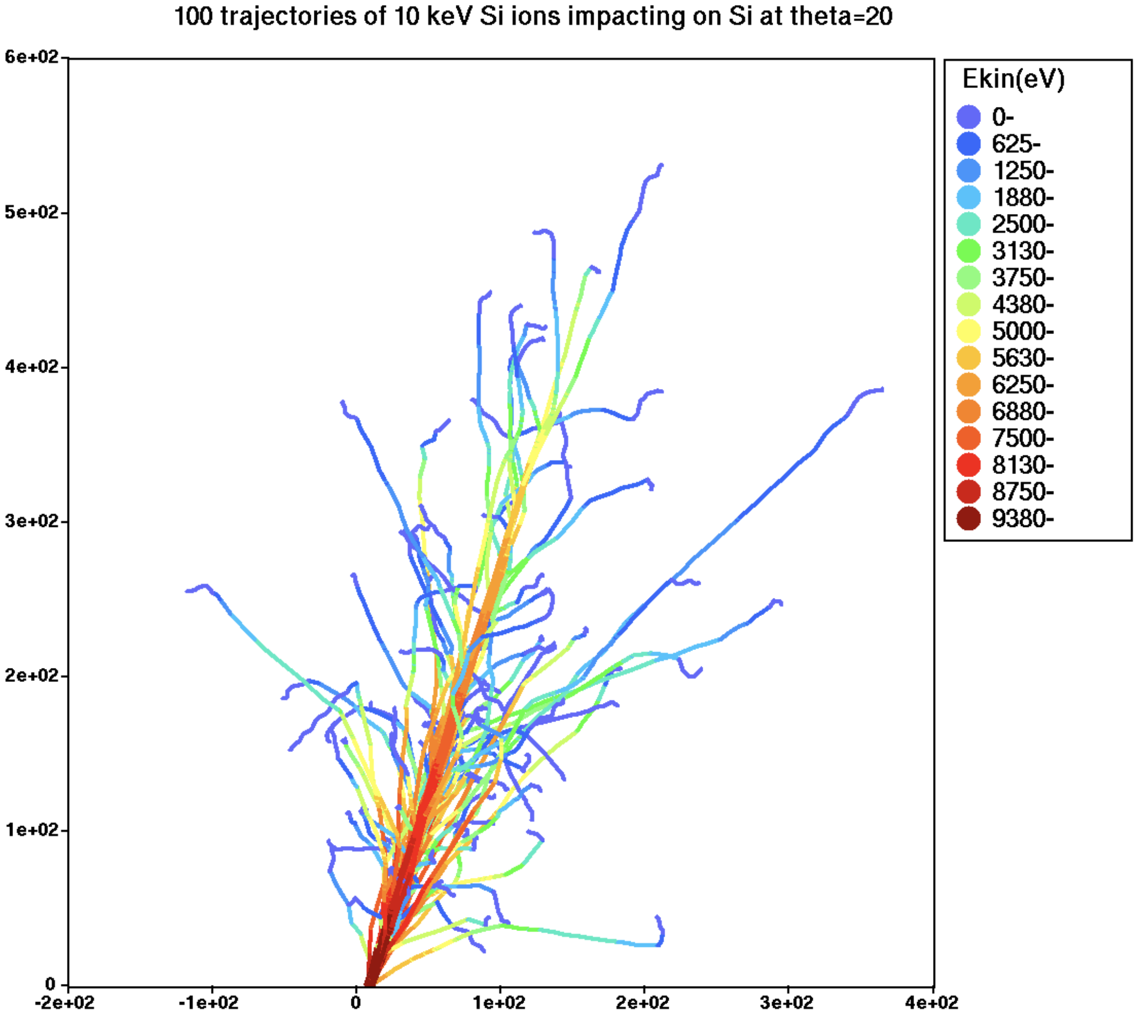
- The calculation:

$$Range = R = \int_0^{E_{max}} \frac{1}{S(E)} dE$$

  is only useful as an estimation of the maximum range, i.e. the range of those ions that happen to travel in a straight path

- For most cases, ions don't travel in a straight path!





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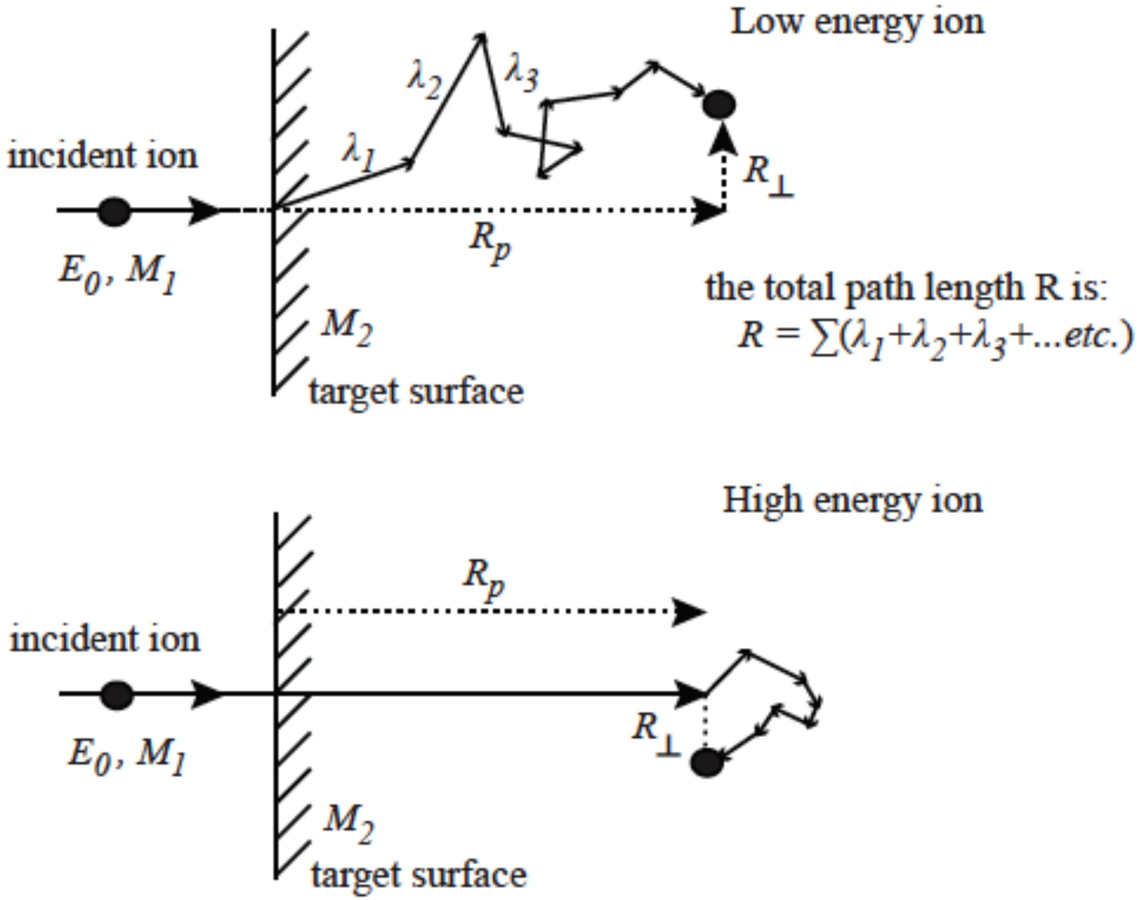
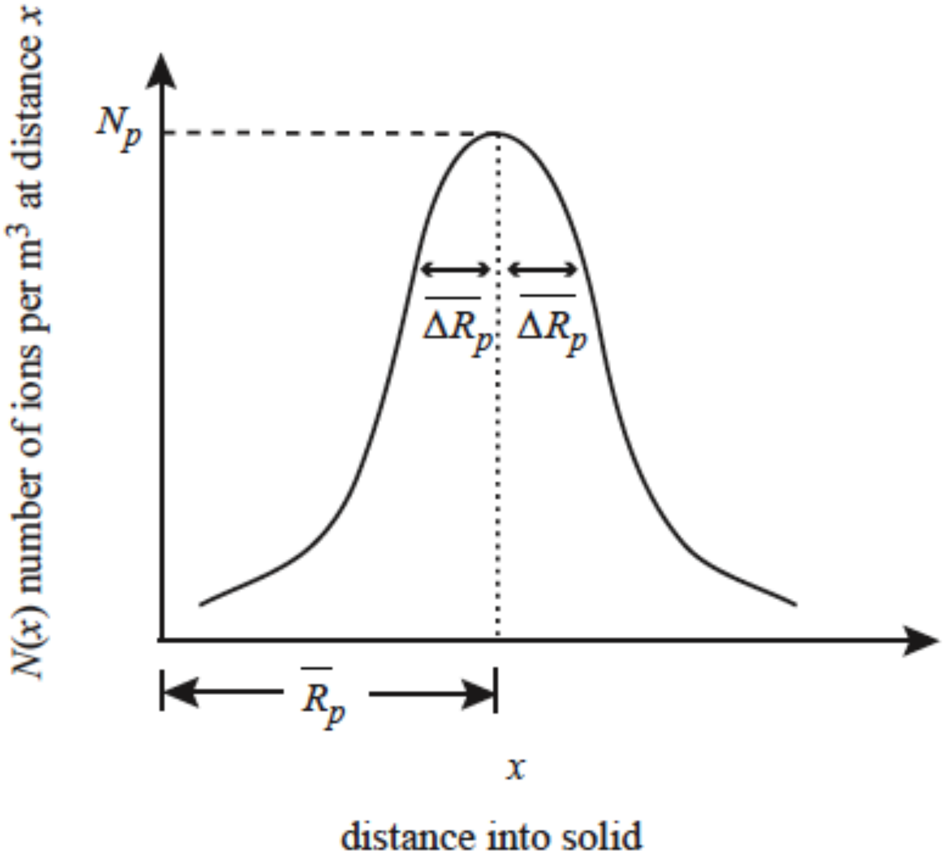
Projected Range - Cases



Concentration

- The stopping positions are distributed according to a Gaussian:



Concentration depends on:

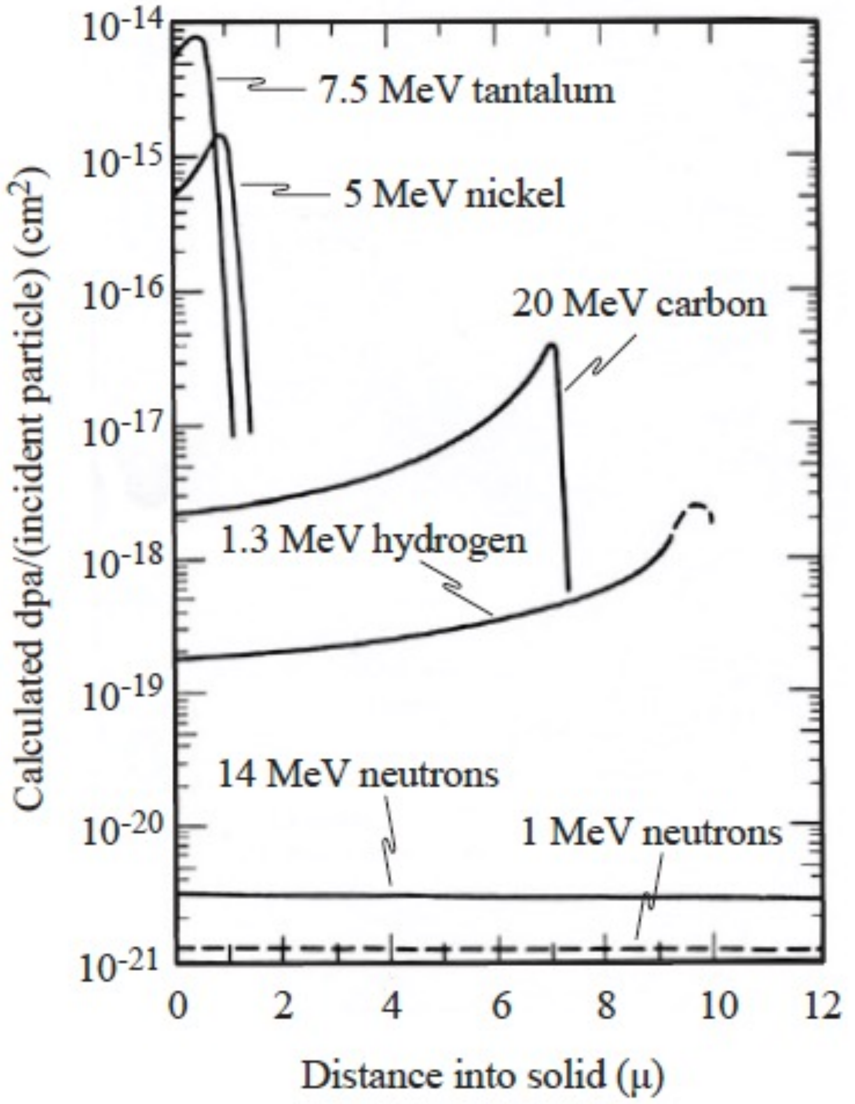
Practical Implications of Range

At low energies where S_n and S_e are comparable, the stopping positions are distribution according to a Gaussian:

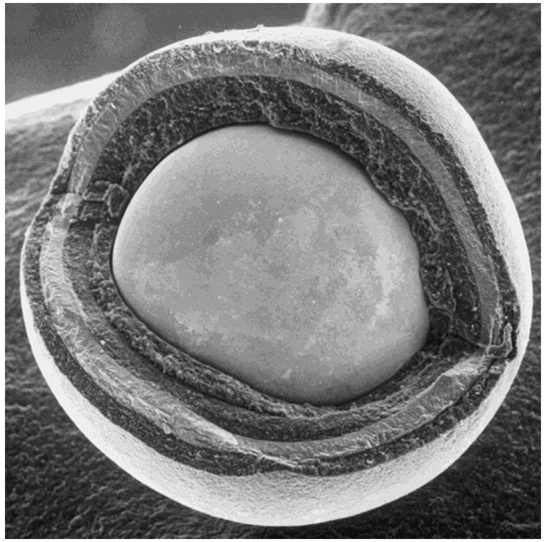
$$N(x) = \frac{0.4N_s}{\Delta R_p} exp\left(-1/2\left\{\frac{x-R_p}{\Delta R_p}\right\}^2\right)$$

Maximum concentration, N_p:

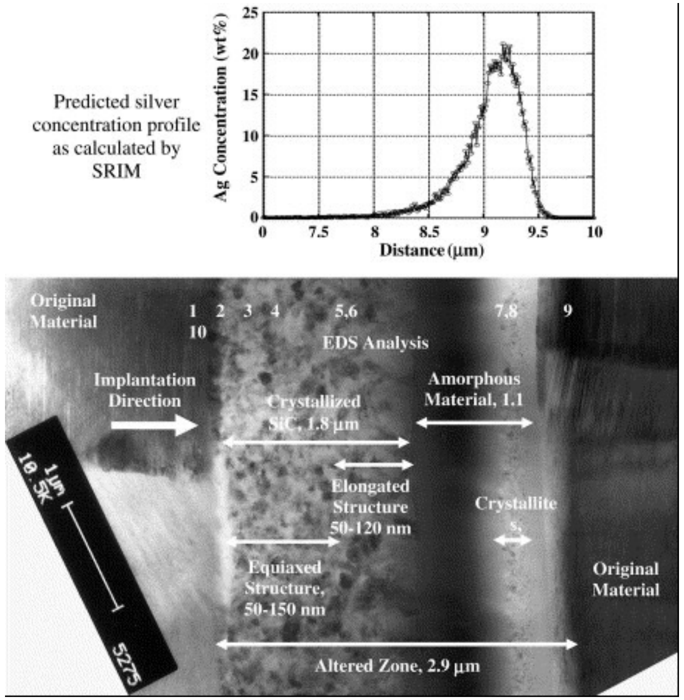
$$N_p \sim \frac{0.4N_s}{\Delta R_p}$$

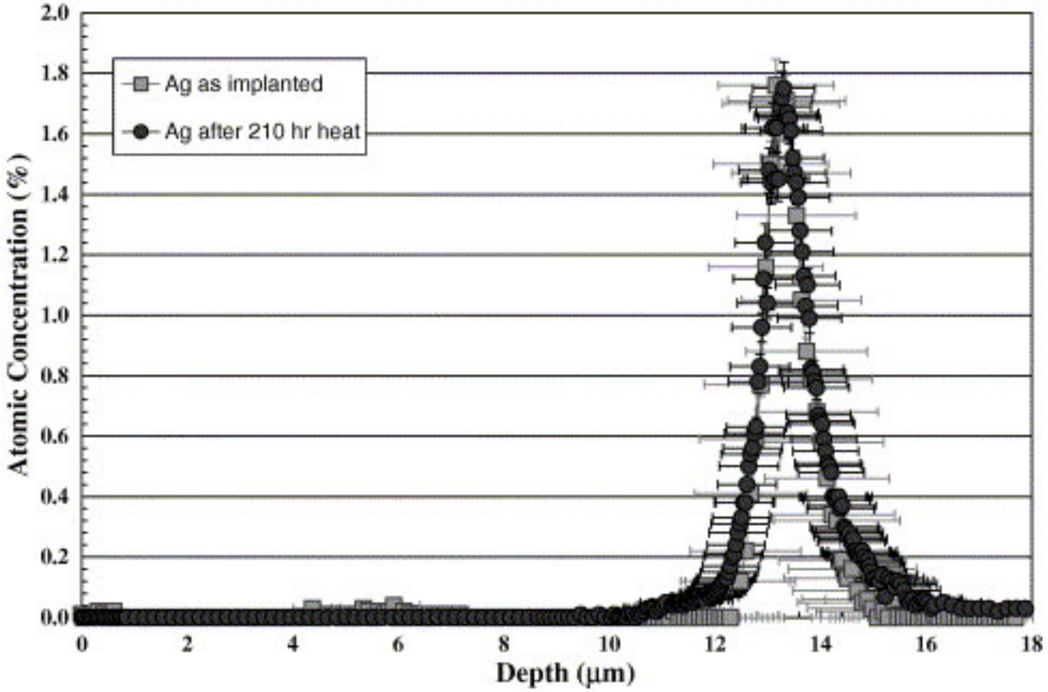


Practical Implications of Range



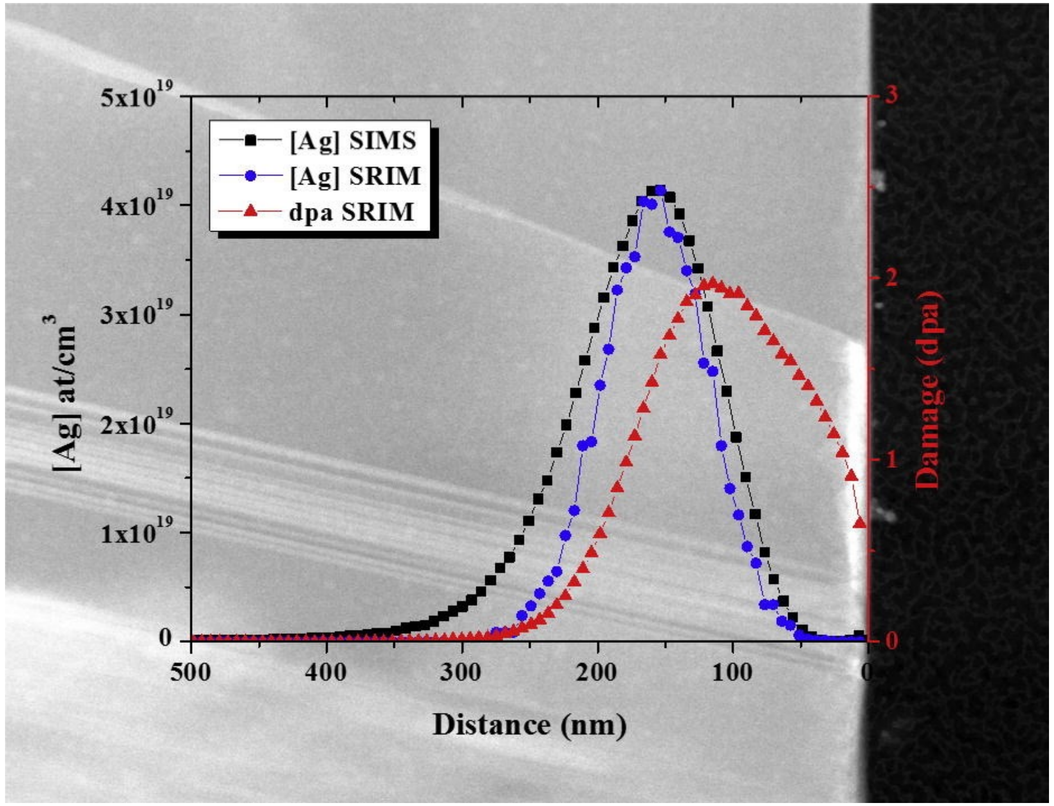
A TRISO fuel particle

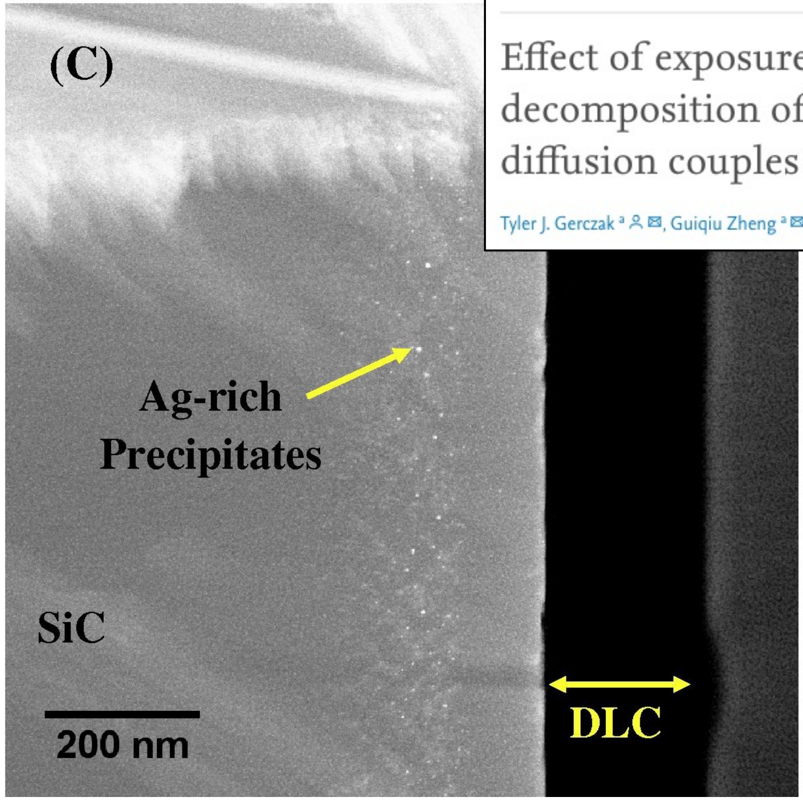




https://doi.org/10.1016/j.jnucmat.2006.05.043

Practical Implications of Range





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Effect of exposure environment on surface decomposition of SiC–silver ion implantation diffusion couples

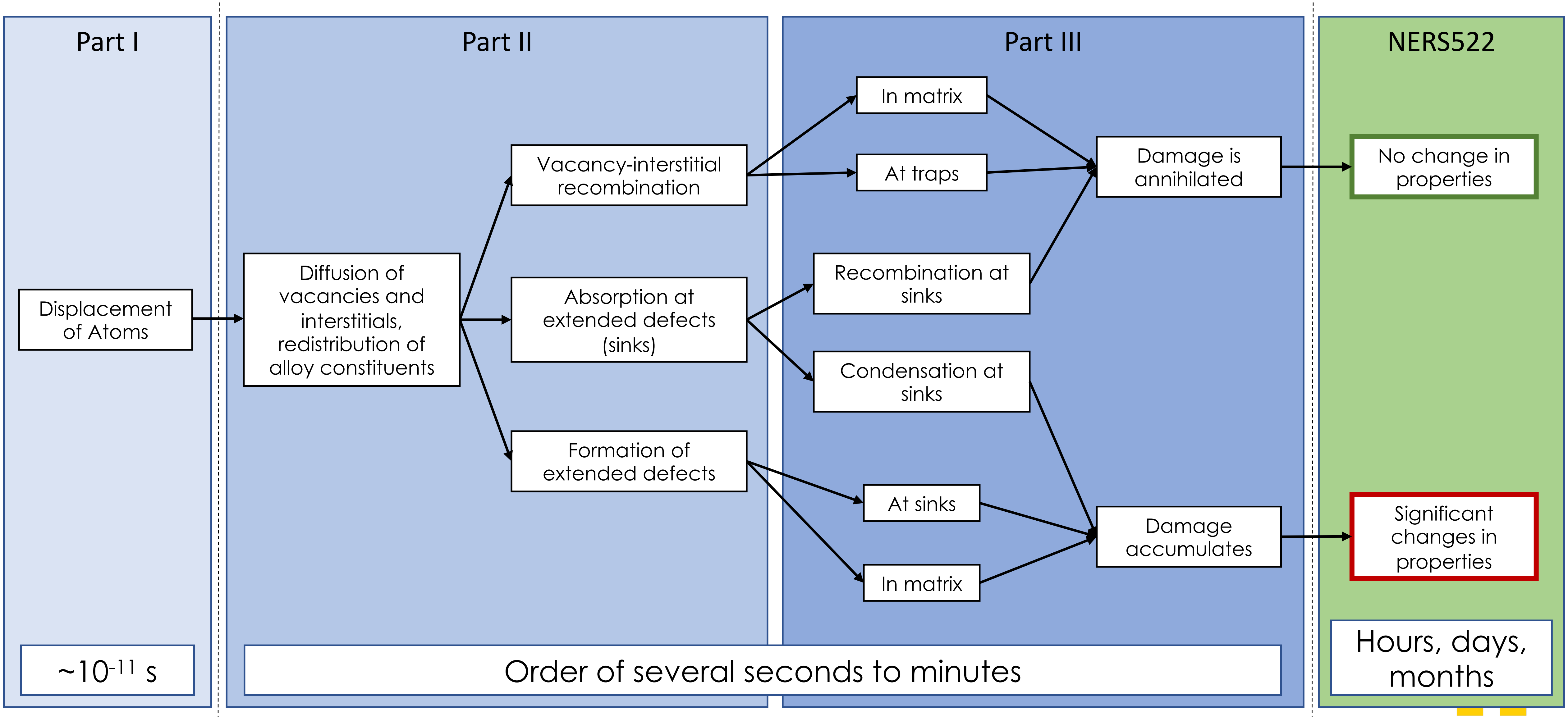
Tyler J. Gerczak [a], Guiqiu Zheng [a], Kevin G. Field [b, 1], Todd R. Allen [c]

10 citations!

https://doi.org/10.1016/j.jnucmat.2006.05.043

In kilograms, what is the weight of the world’s heaviest potato?

Flow chart for radiation damage



Louis Mansur, "Mechanisms & Kinetics of Radiation Effects in Metals and Alloys", in: Kinetics of Nonhomogeneous Processes, 1987

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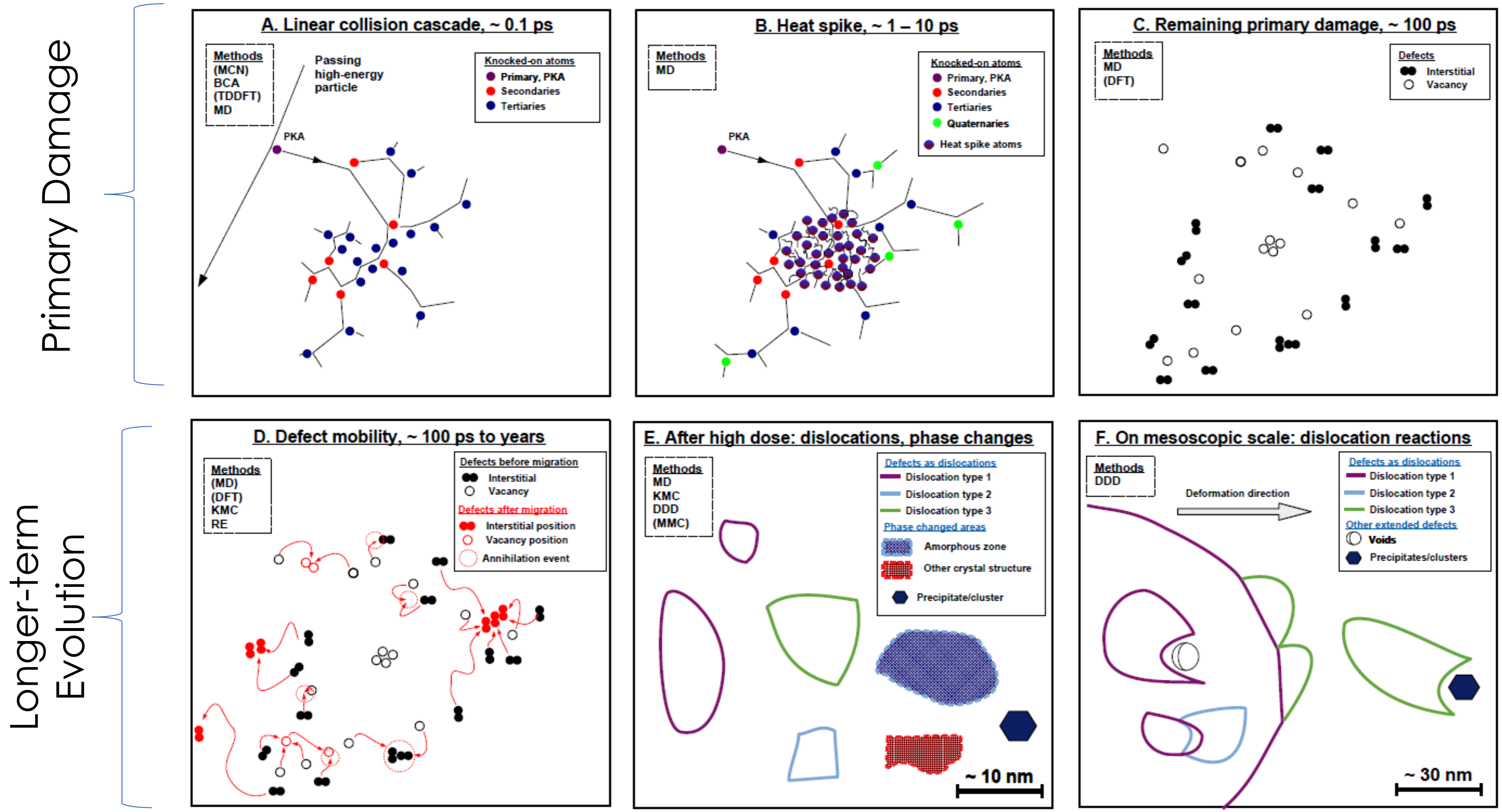
A visual of that flow chart:



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Displacement of Atoms in Detail

Part I

Displacement of Atoms

(Radiation Damage Event)

$\sim 10^{-11}$ s

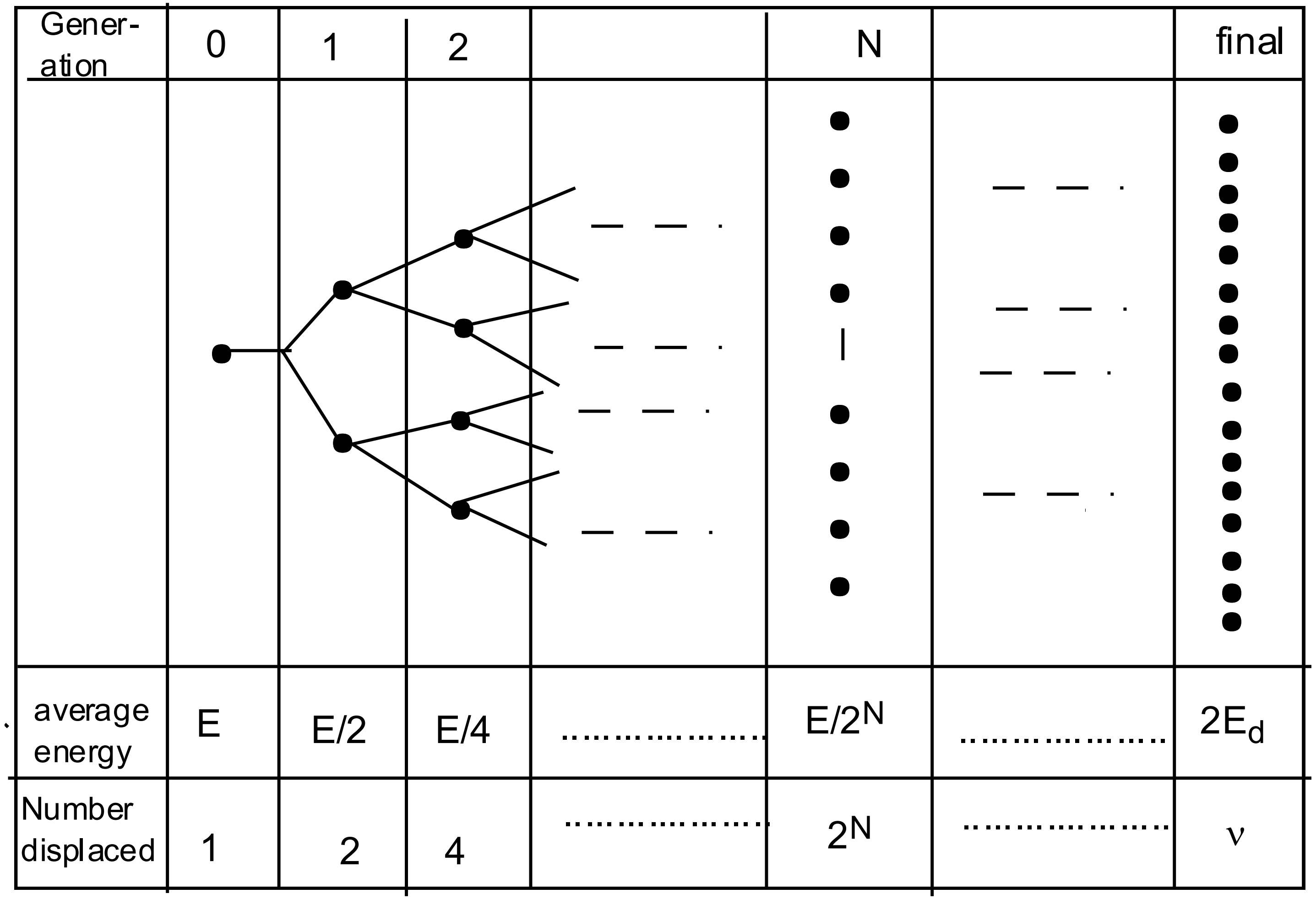
Displacement of atoms is primarily evaluated as the **primary radiation damage event** which is composed of the following sequence of events:

1. The *interaction* of an energetic particle with a lattice atom
2. The *transfer of kinetic energy* to the lattice atom resulting in the primary knock-on atom (PKA)
3. The *displacement* of the lattice atom from it's lattice site
4. The *passage* of the displaced atom through the structure and the potential accompanying creation of additional knock-on atoms
5. The *production of a displacement cascade*
6. The *termination of the PKA* as an interstitial in the structure

When does a cascade end?

- Remember:

- Cascade ceases when knock-on energy is:



K-P Model

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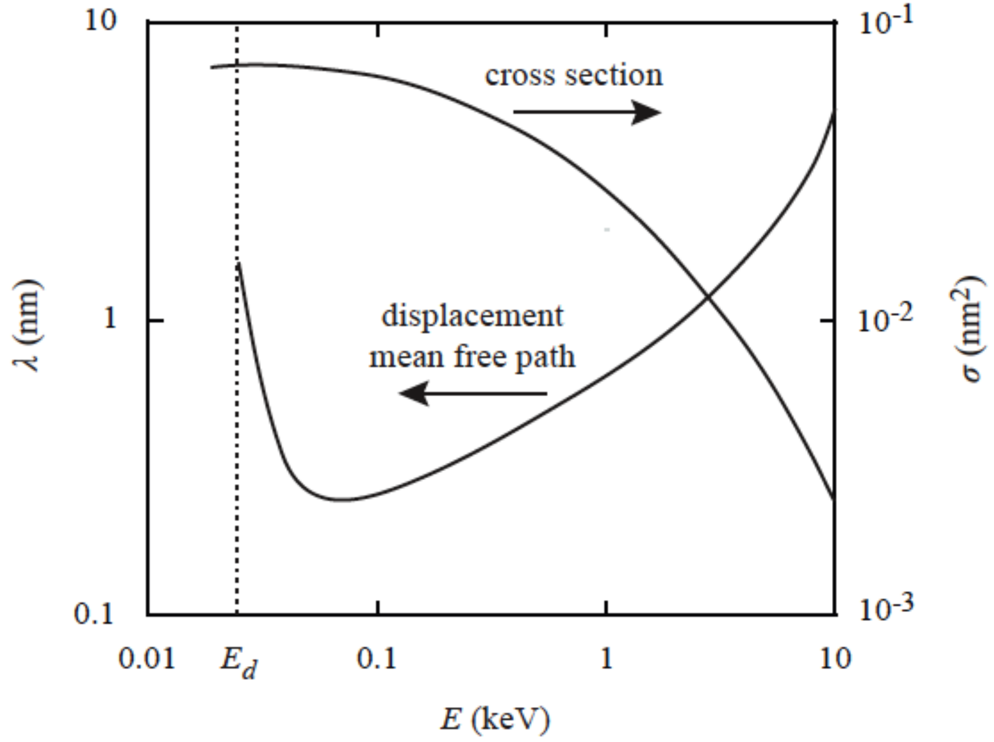
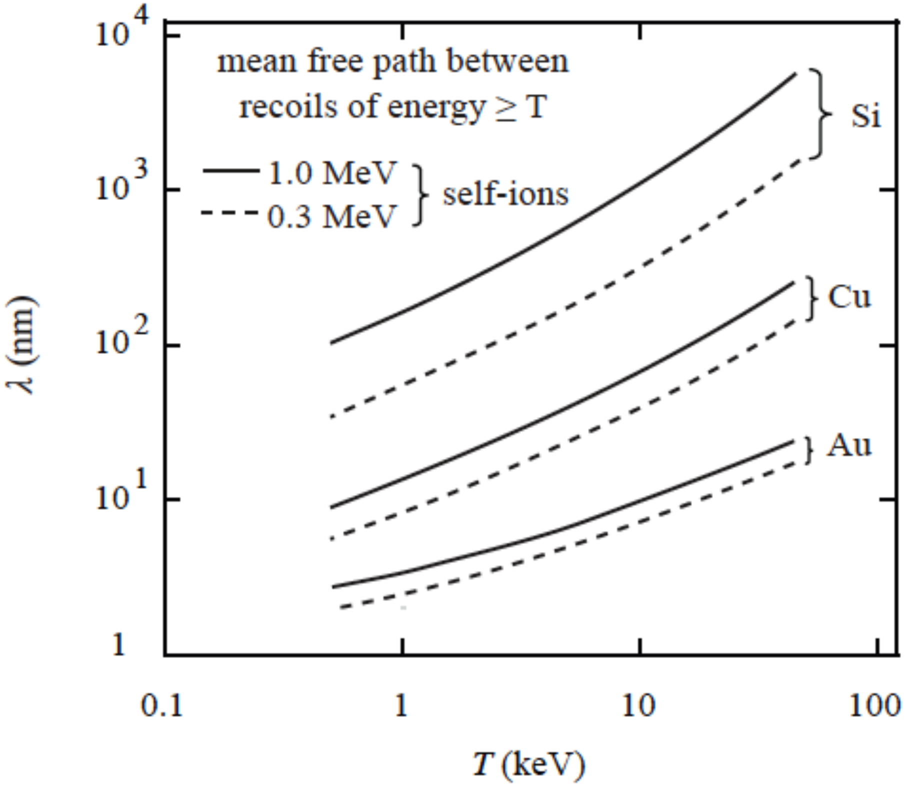
Mean free path between recoils

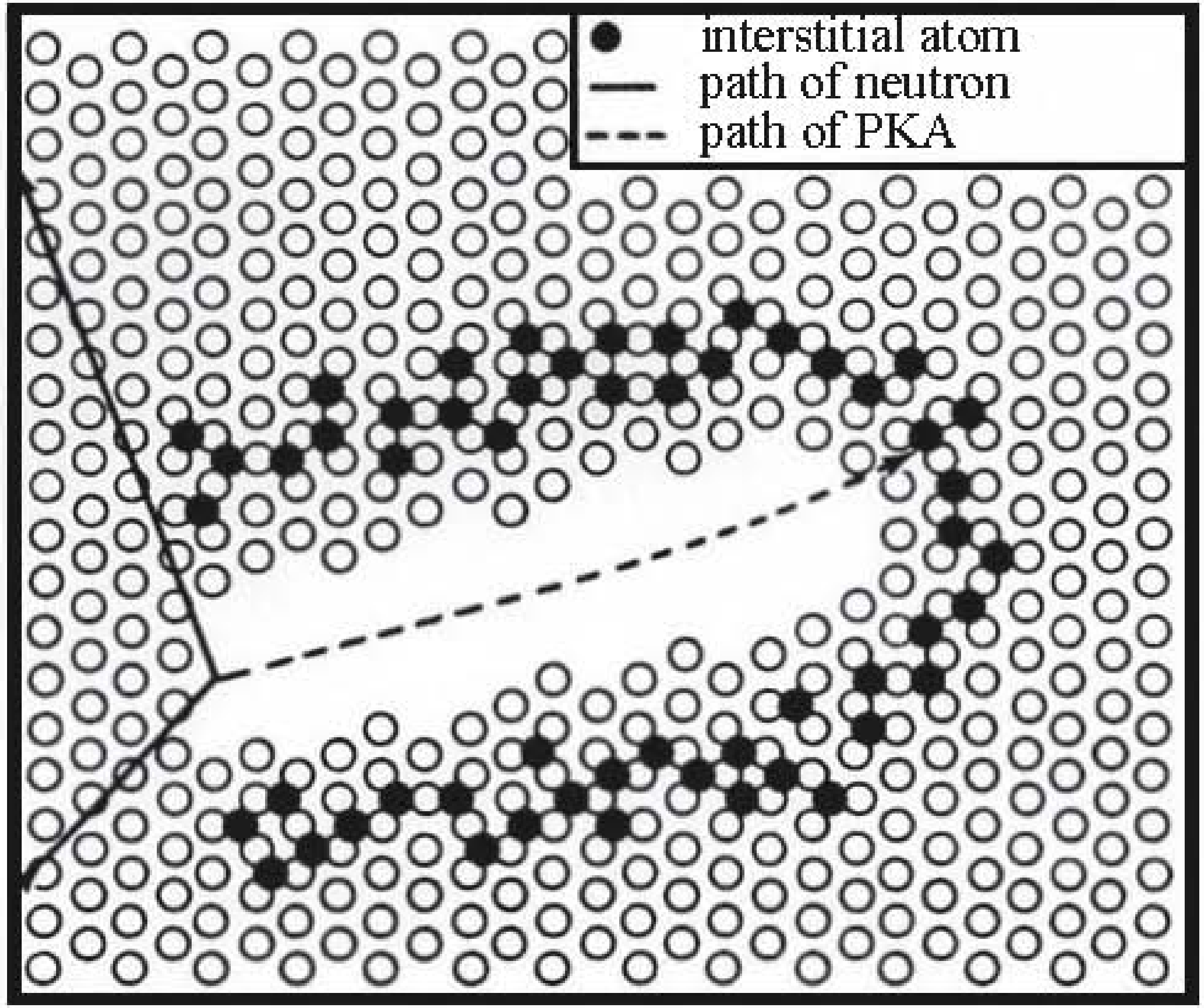
- Brinkman calculated the mean free path, determined spacing approached atomic separation distances.
  - Led to the realization that many cascades are not a collection of isolated Frenkel pairs





Original conception of the damage cascade

Use the term "damage cascade" to signify the continued damage effects from PKA, SKA, etc…



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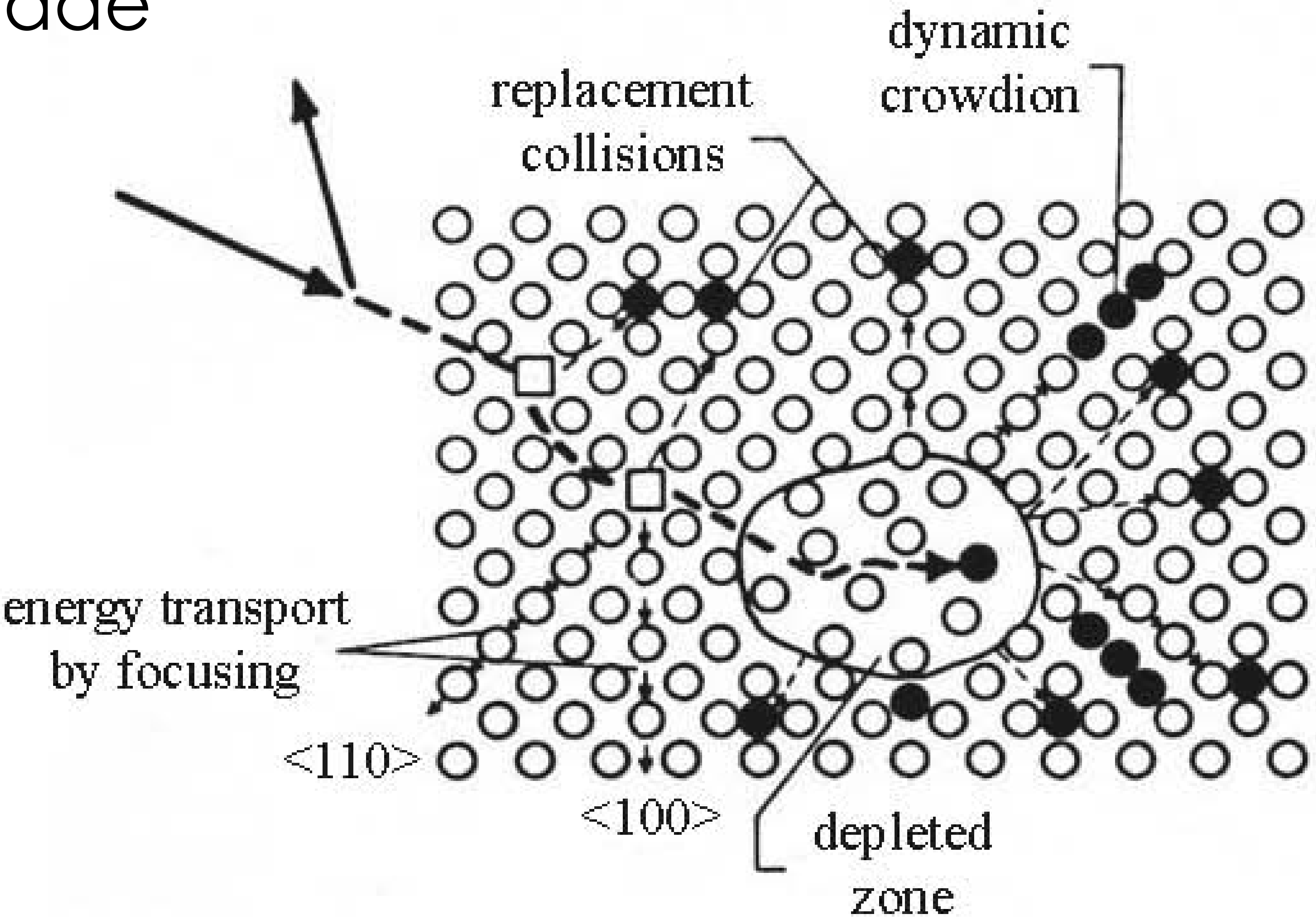
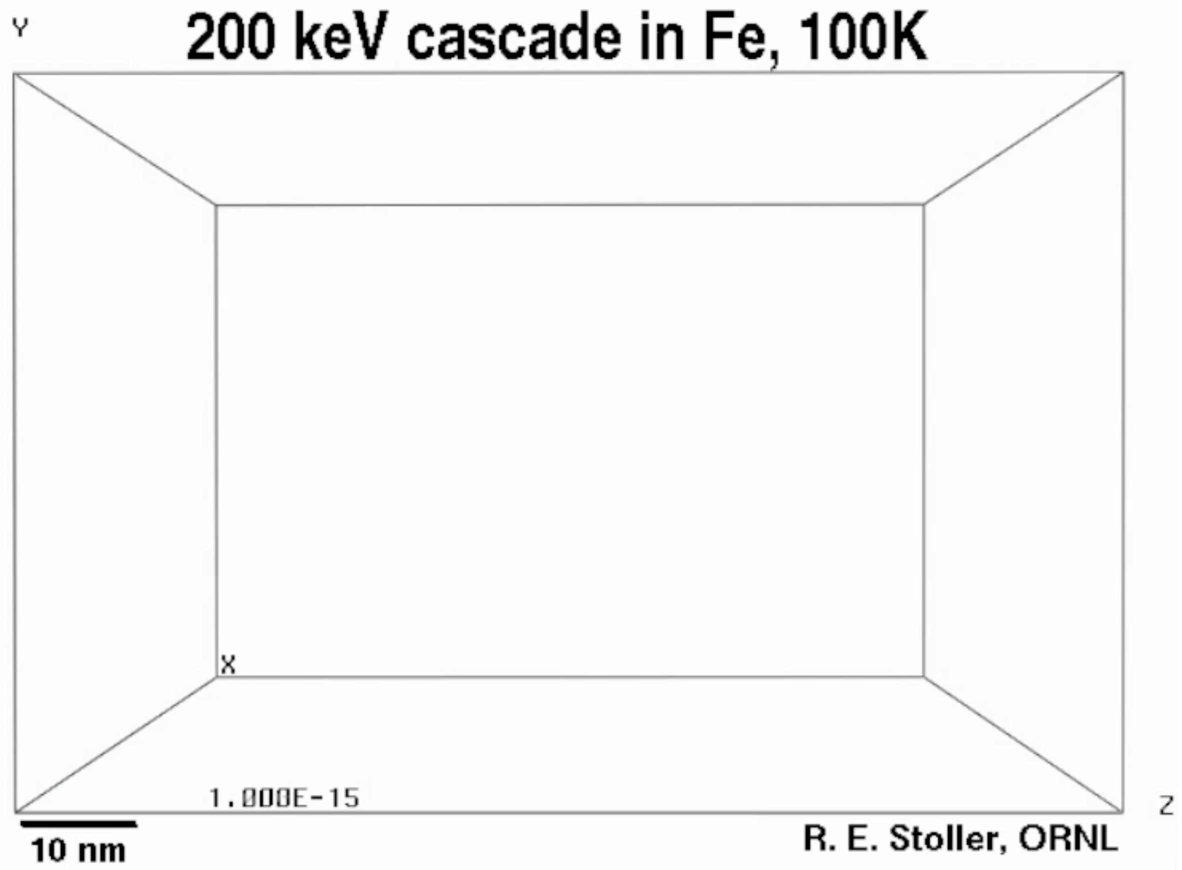
Another revised conception of the damage cascade

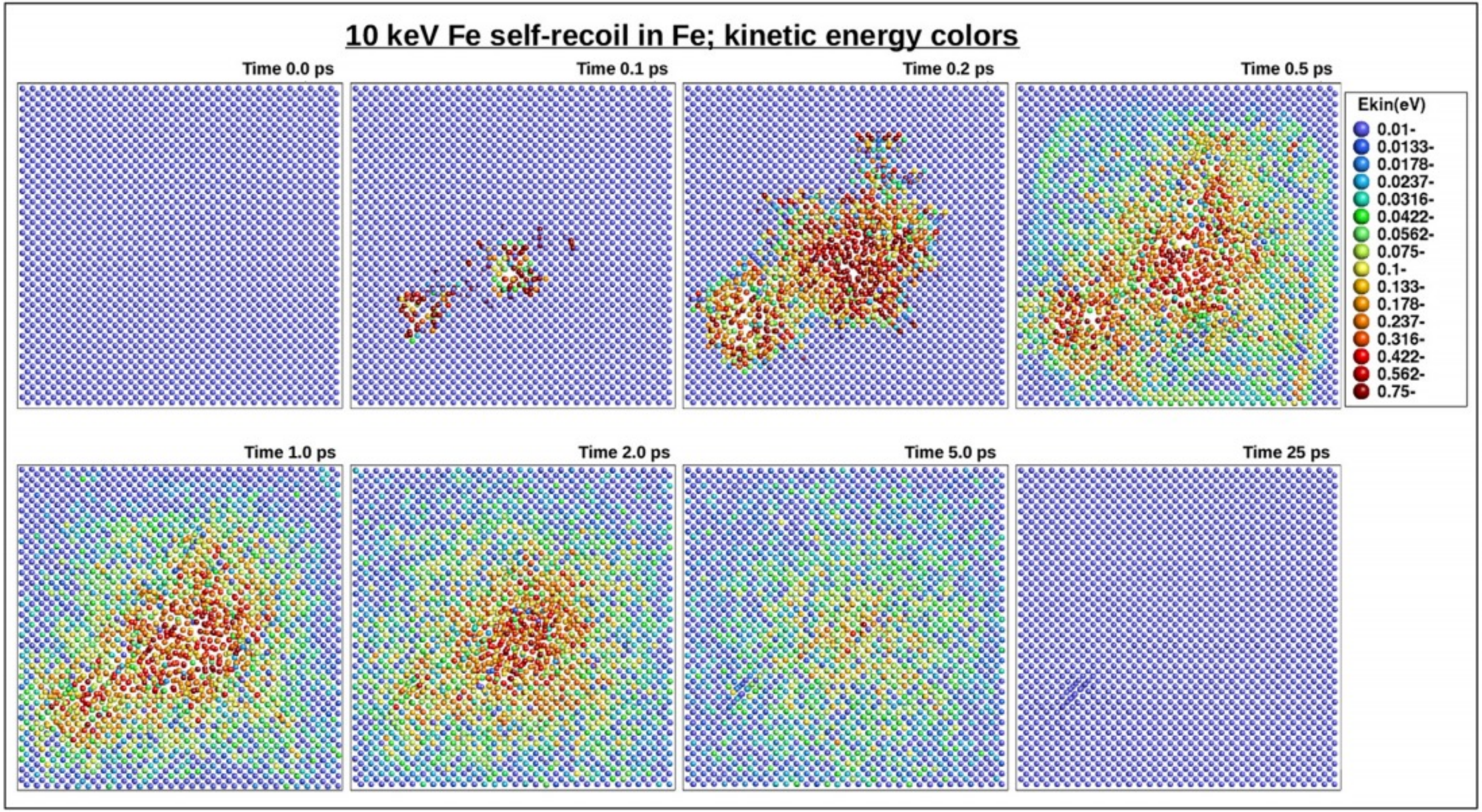


A more realistic visual:

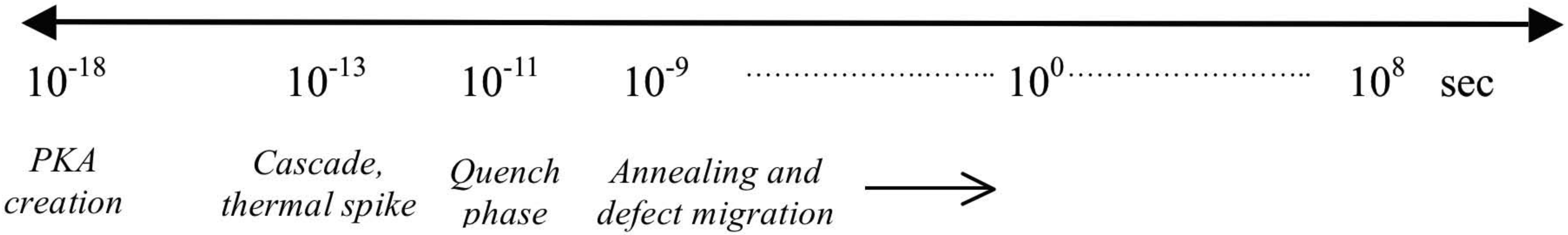
3.1 Molecular Dynamics (MD) simulation of the development of a cascade from a 20 keV recoil in iron at 100K. Note the striking difference in defect density between the peak of the ballistic regime (~1 ps) and that at the end of the quench (~5 ps). (courtesy, R. Stoller, Oak Ridge National Laboratory)



Visual snapshot of a cascade and stages

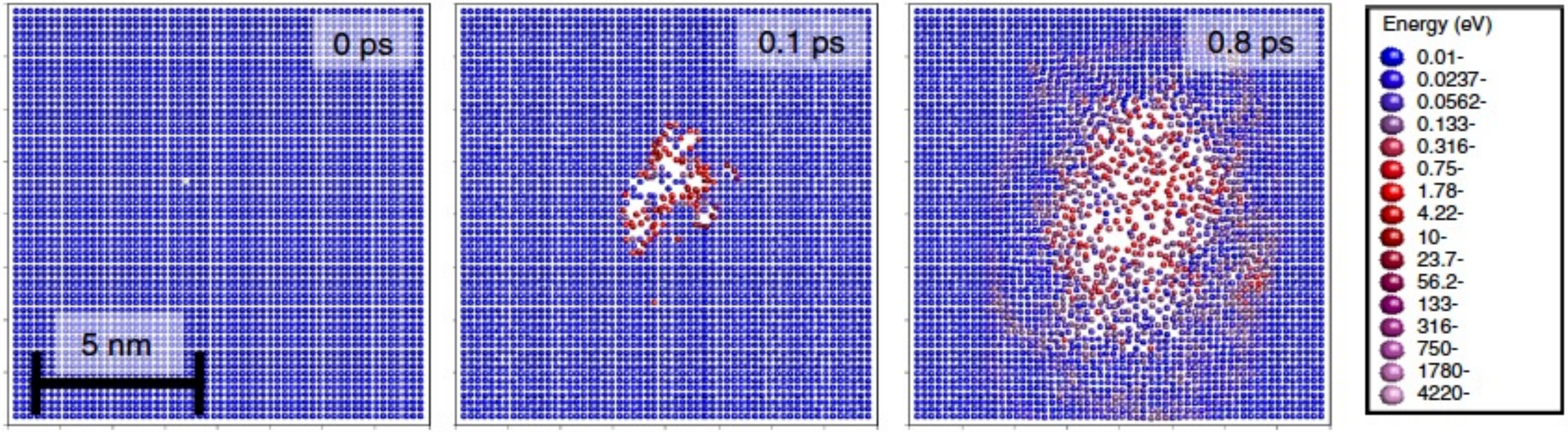


Cascades have four distinct stages:



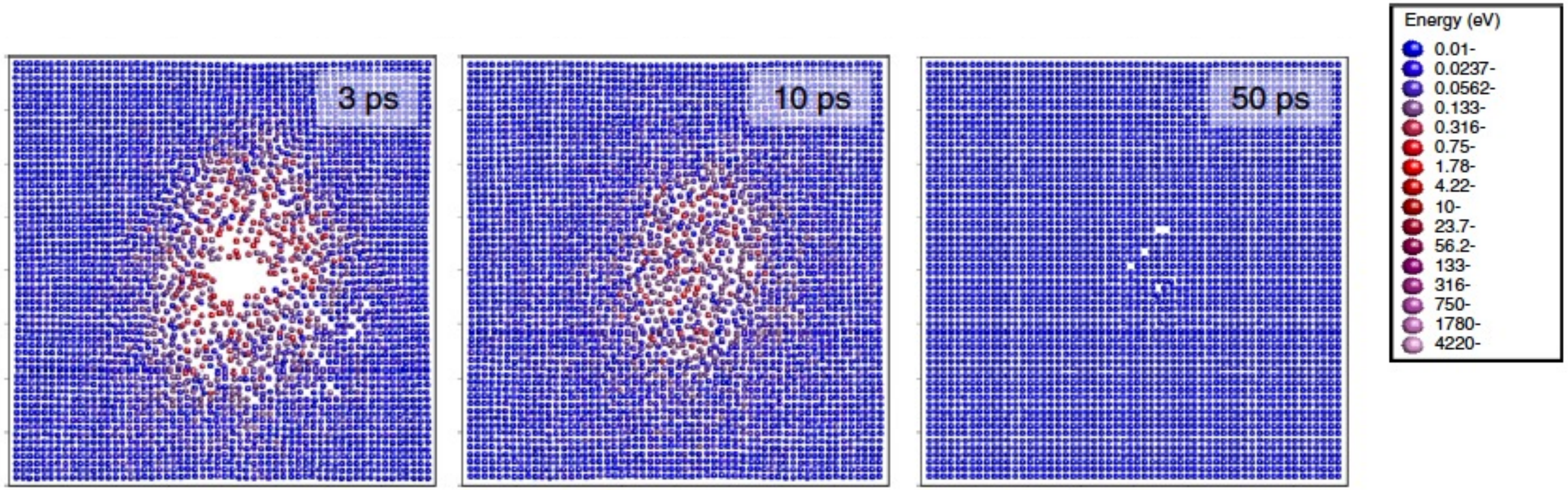
1. Collisional
2. Thermal spike
3. Quenching
4. Annealing

Collisional -> Thermal Spike



- Energy transfer below displacement energy (E_d) heats lattice
- Local temperature can exceed melting point (T_m)

Quenching -> Annealing



- The thermal spike cools quickly (ps time scale) causing rapid recrystallization from a hot liquid
- The recrystallization process drives toward "repair" causing the displaced defect pairs (interstitials and vacancies) to recombine
  - Does not require thermally activated defect migration
  - If recrystallization front moves quickly -> isolated vacancies
- Remaining defects may exist, and given enough energy in the system (e.g. elevated temperature) they may be mobile leading to additional annealing

Quenching -> Annealing

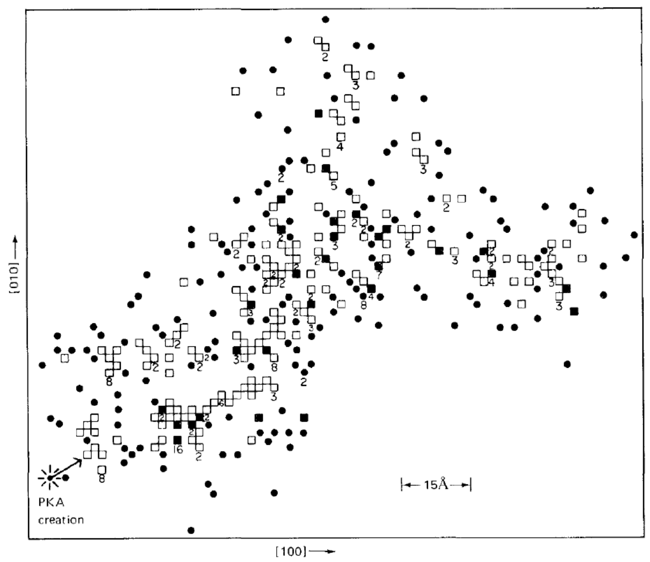


Fig. 17.27 Displacement spike due to a 20-keV PKA in iron projected onto the (001) plane (0°K). [After J. R. Beeler, Jr., *Phys. Rev.*, 150: 470 (1966).]

800k anneal

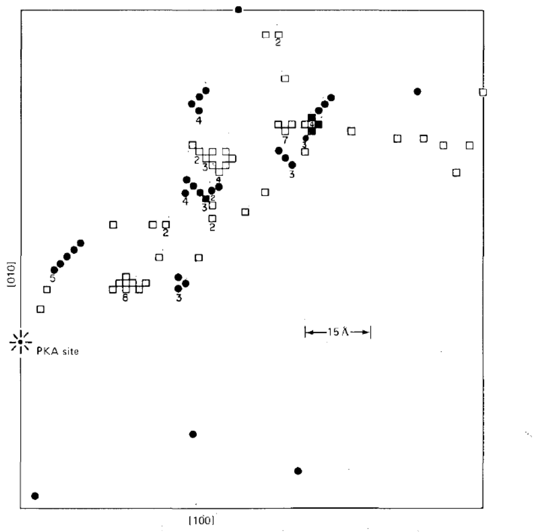
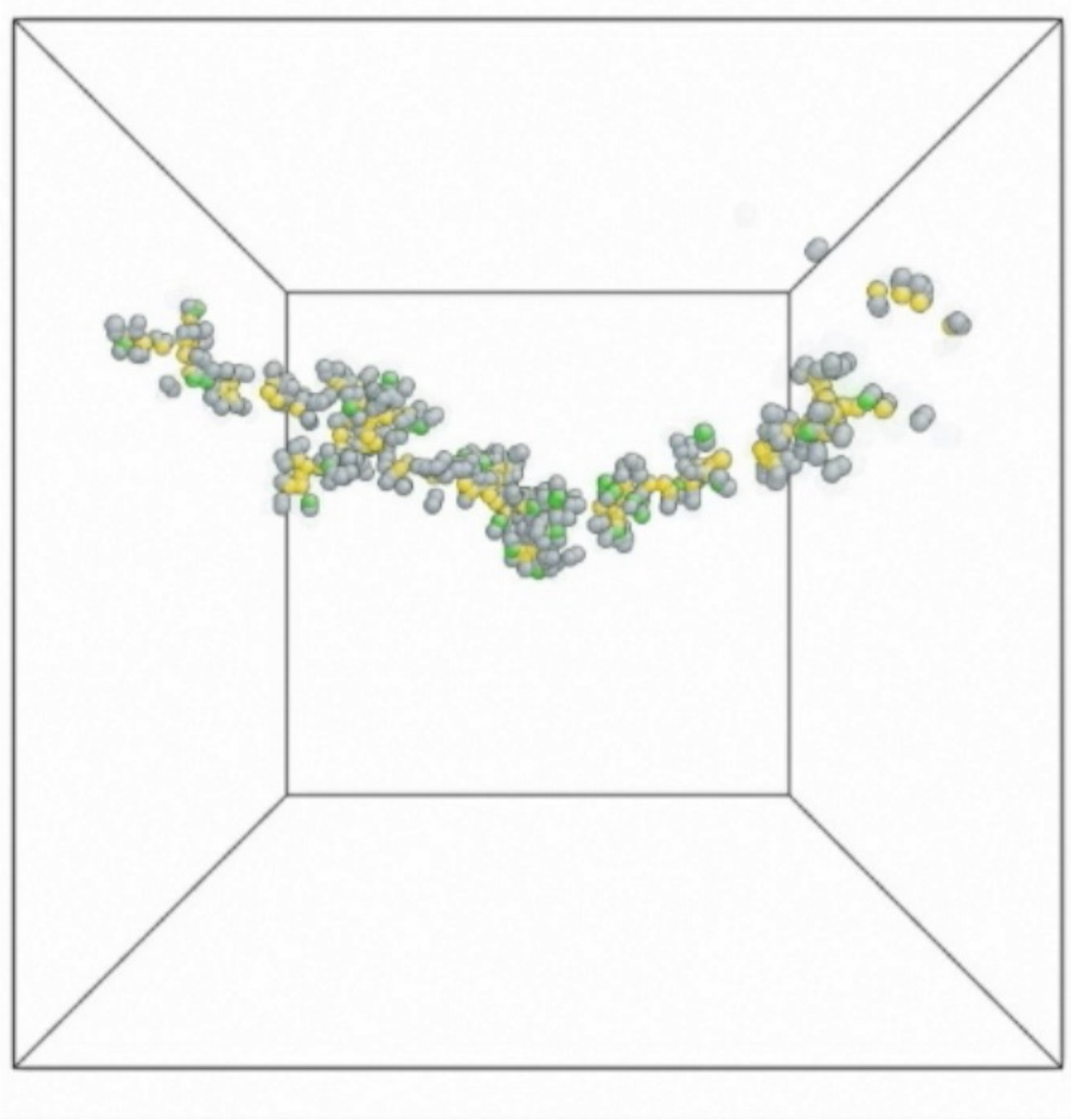


Fig. 17.28 Displacement spike [projected onto the (001) plane] due to a 20-keV PKA in iron after annealing at 800°K (6000 interstitial jumps and 60 vacancy jumps). The preannealed spike is shown in Fig. 17.27. Numbers on the diagram denote cluster sizes. Twelve interstitials have migrated outside the range of the diagram and are not shown. (After Ref. 29.)

- Annealing can be simply evaluated by looking at the jump rate, where insterstials are enabled to jump to different lattice sites more frequently. The following possibilities can happen:
  - Point defect jumps into a recombination volume around a point defect of opposite sign -> the two are annihilated
  - A point defect jumps near a cluster of same sign defects -> cluster grows by 1
  - A point defect jumps near a cluster of opposite sign defects -> cluster shrinks by 1

A more realistic visual:

3.3 Cascade formation and cooling in an Fe-10% Cr alloy, In this MD simulation, the yellow spheres are vacancies, the grey are iron interstitials and the green are chromium interstitials. Chromium is modeled as the larger solute, and after cooling, the remaining interstitial population is predominantly iron atoms as their distortion of the lattice is less than that from the oversized chromium atoms. (courtesy, B. Wirth, University of California, Berkeley)



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Questions?