Damage Cascade

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Where we left off last time…

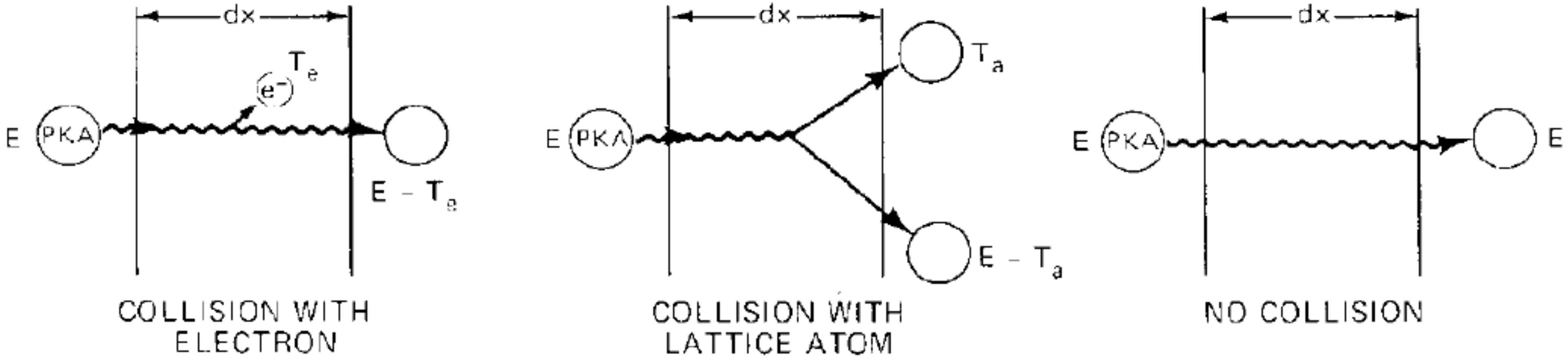


Fig. 17.10 Possible fates of a PKA on passing through a thickness dx of solid.

- To accurately describe the slowing down process, we would need to piece together many potentials depending on closest point of approach
- As an approximation, we divide into two regimes
  - Distant collisions where interactions with electrons dominate
  - Close collisions where nuclei interact

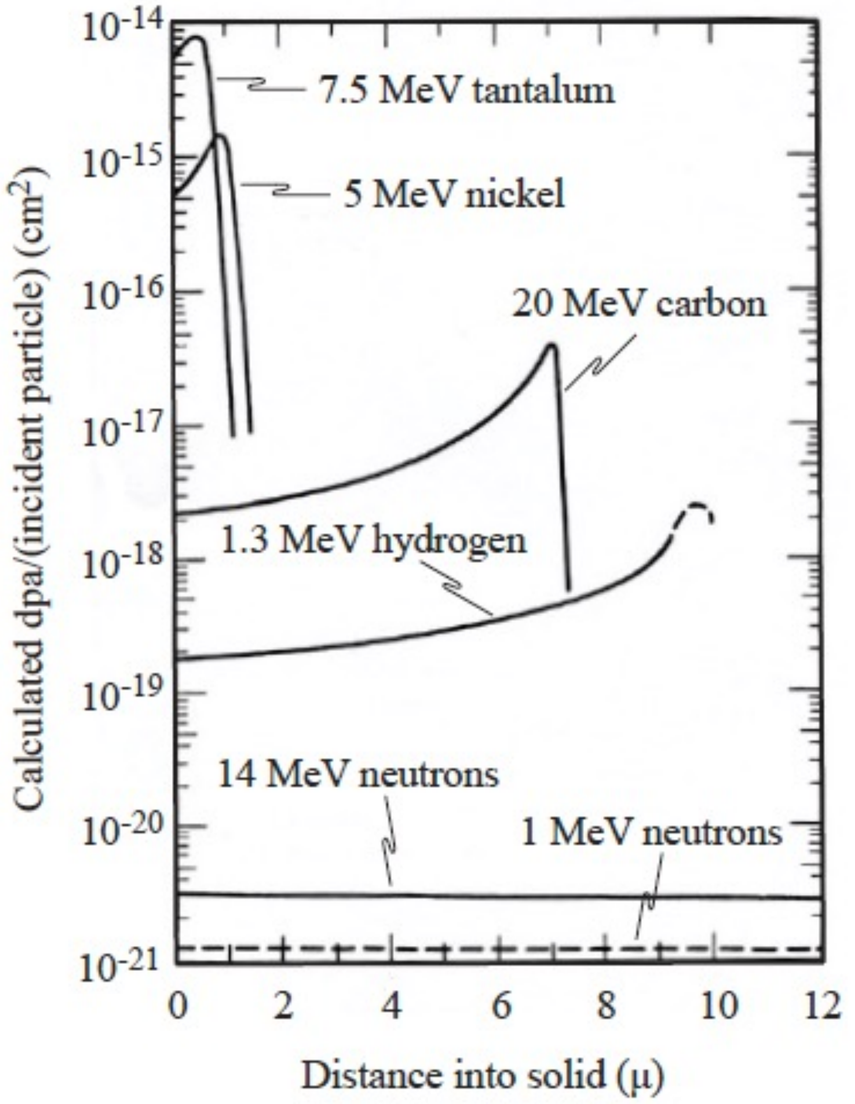
Practical Implications of Range

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:

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



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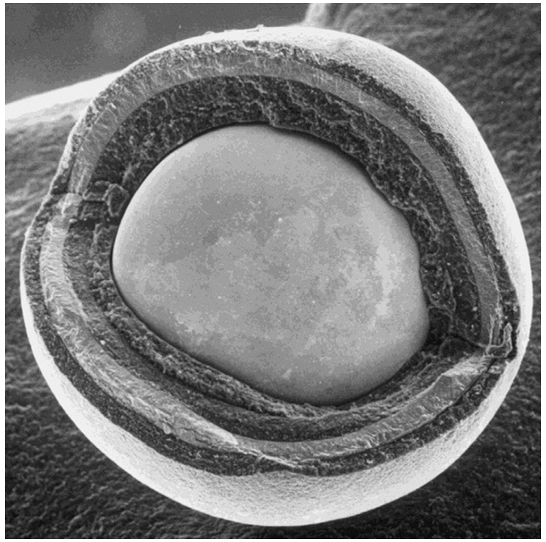
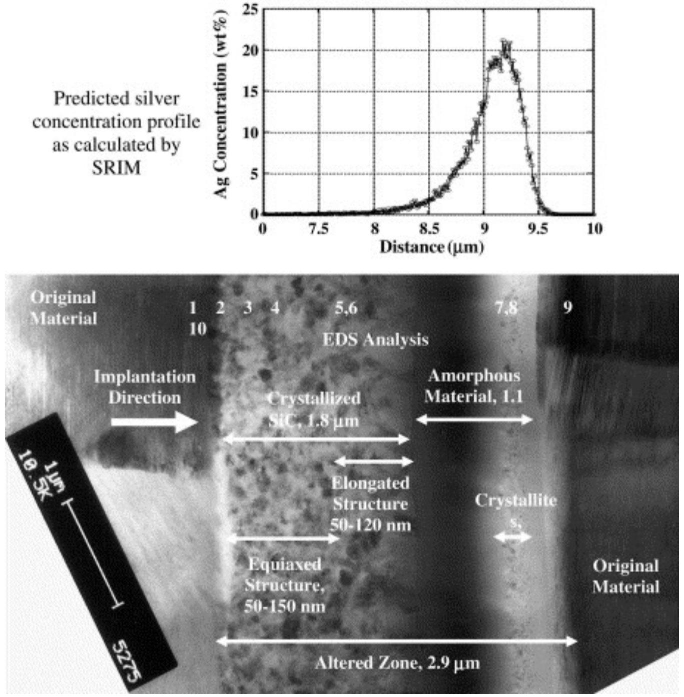
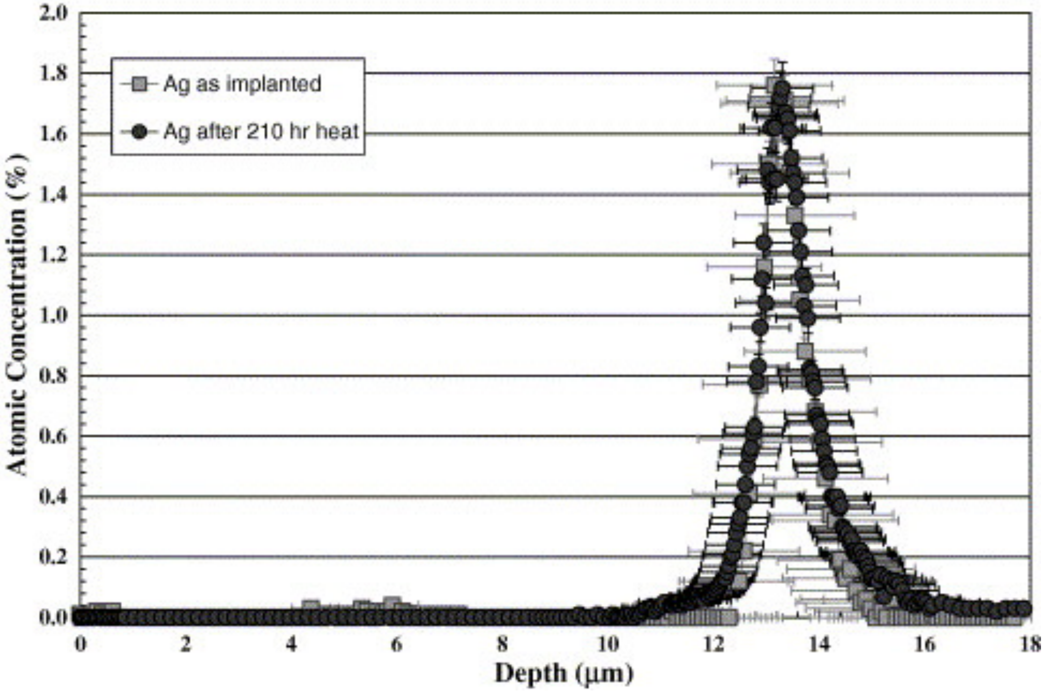
Practical Implications of Range



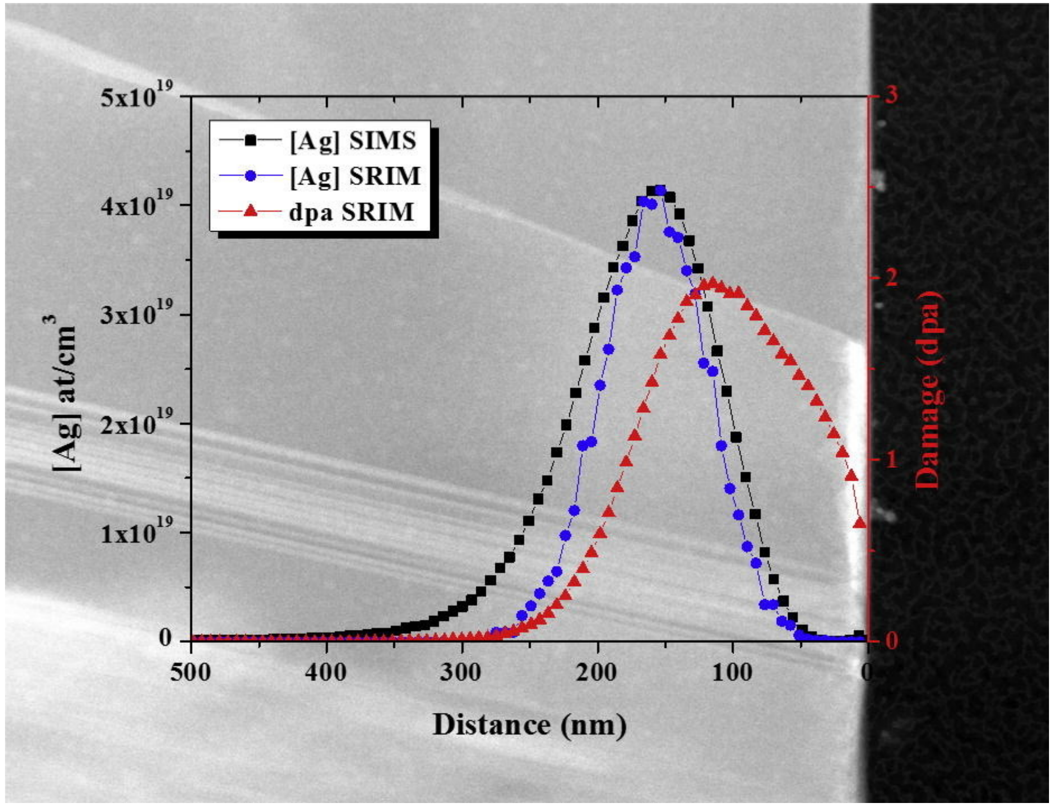
A TRISO fuel particle

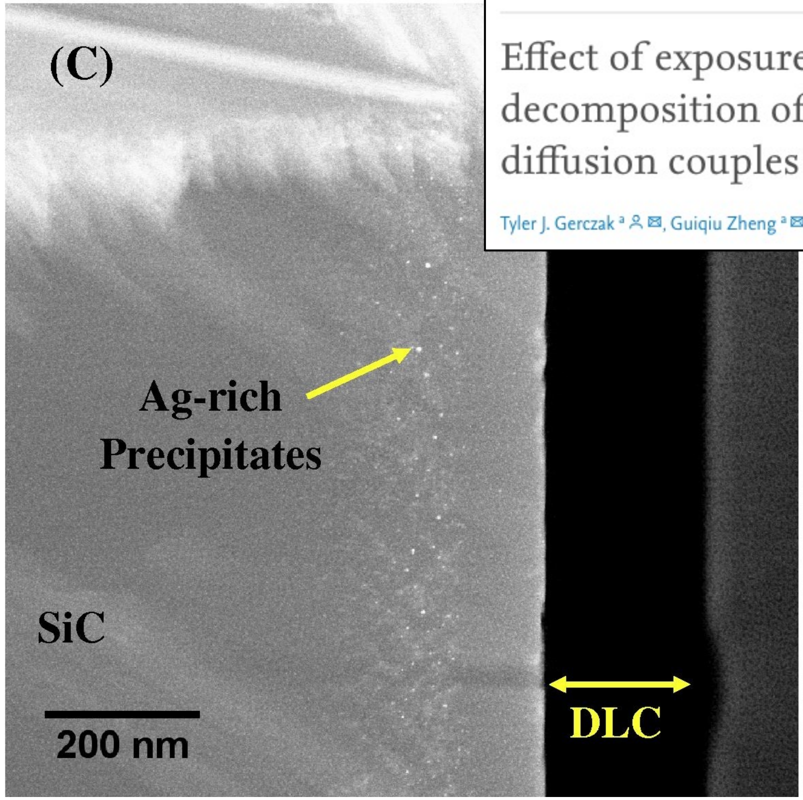




https://doi.org/10.1016/j.jnucmat.2006.05.043

Practical Implications of Range





ELSEVIER
Journal of Nuclear Materials
Volume 456, January 2015, Pages 281-286

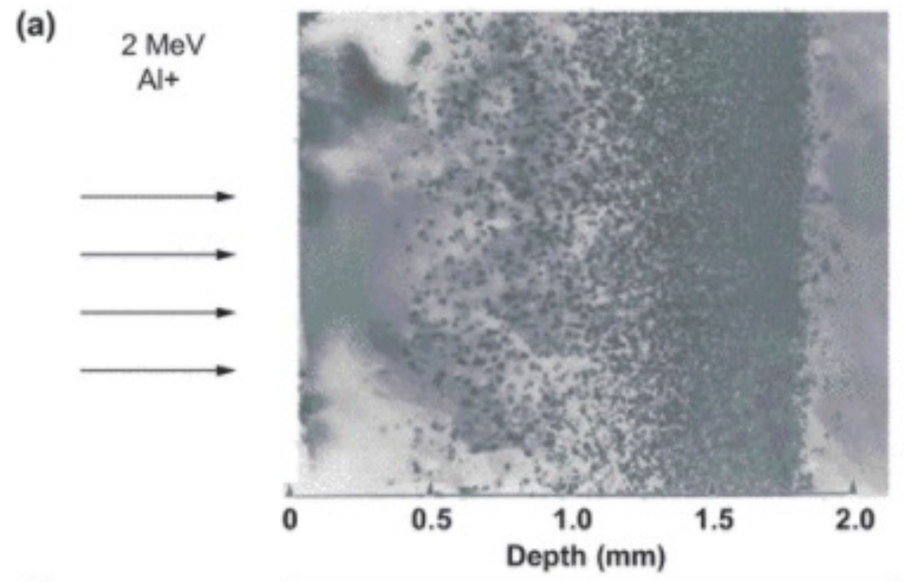
Effect of exposure environment on surface decomposition of SiC–silver ion implantation diffusion couples

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

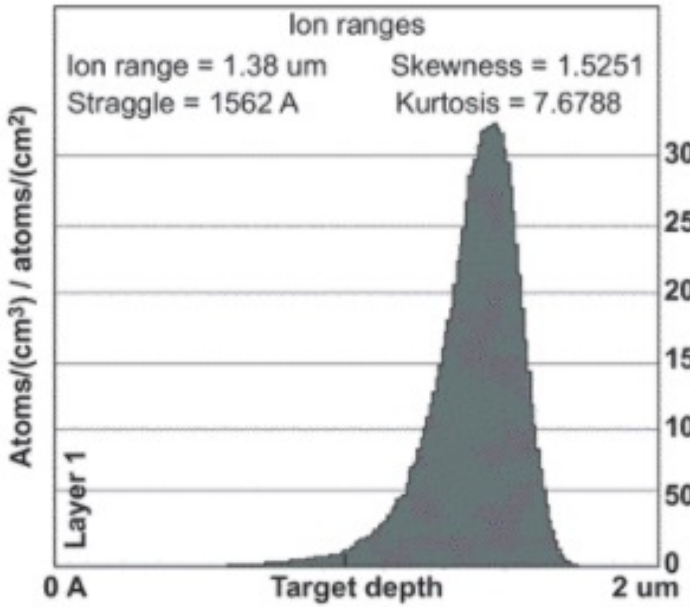
10 citations!

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

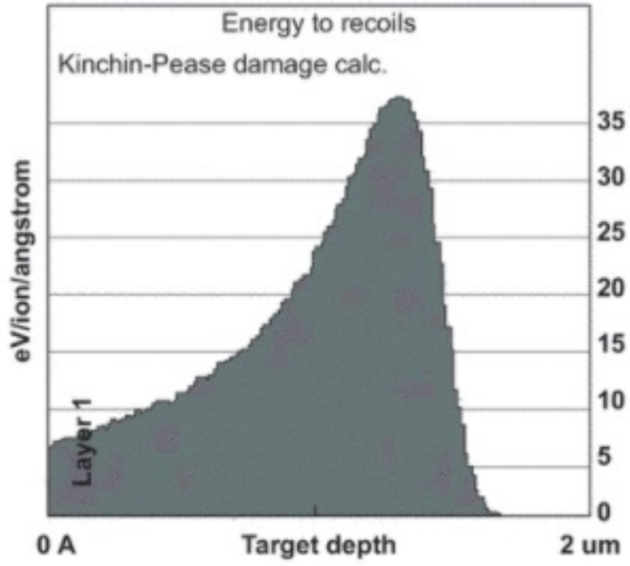
Practical implications of range



Microstructure



Ion Range



Damage Range

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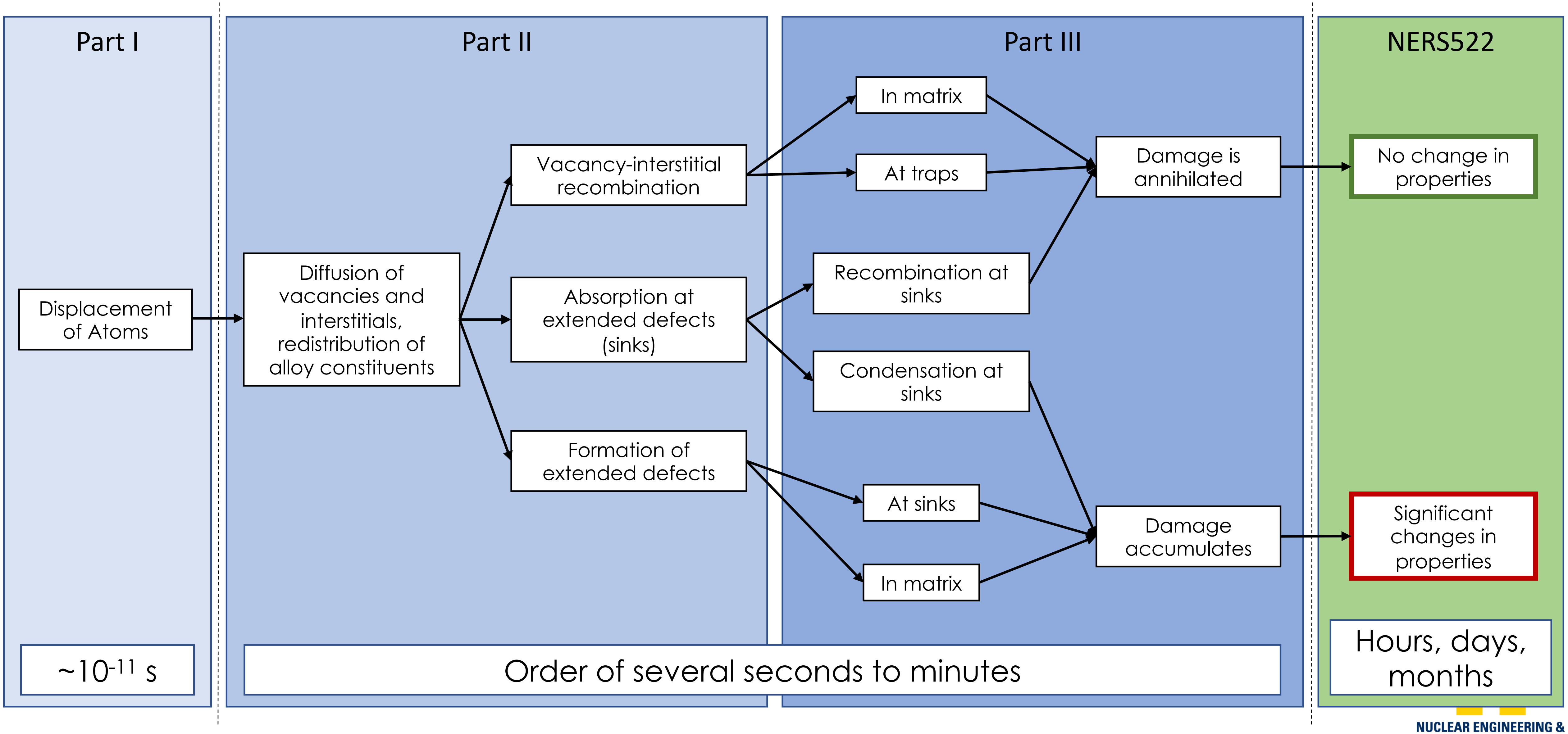
Flow chart for radiation damage



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

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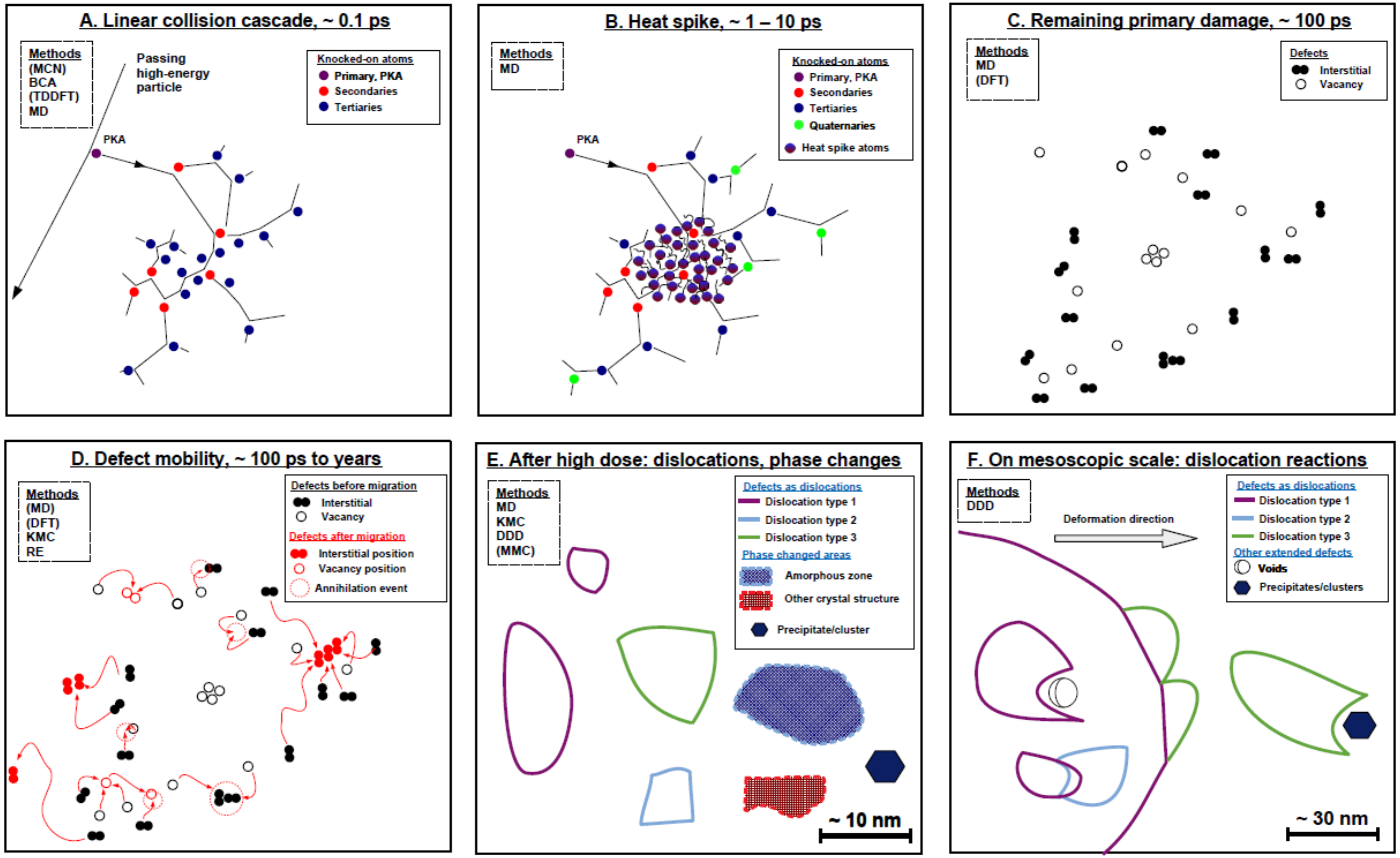
A visual of that flow chart:

Primary Damage

Longer-term Evolution



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Displacement of Atoms in Detail

Part I

Displacement of Atoms

(Radiation Damage Event)

~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

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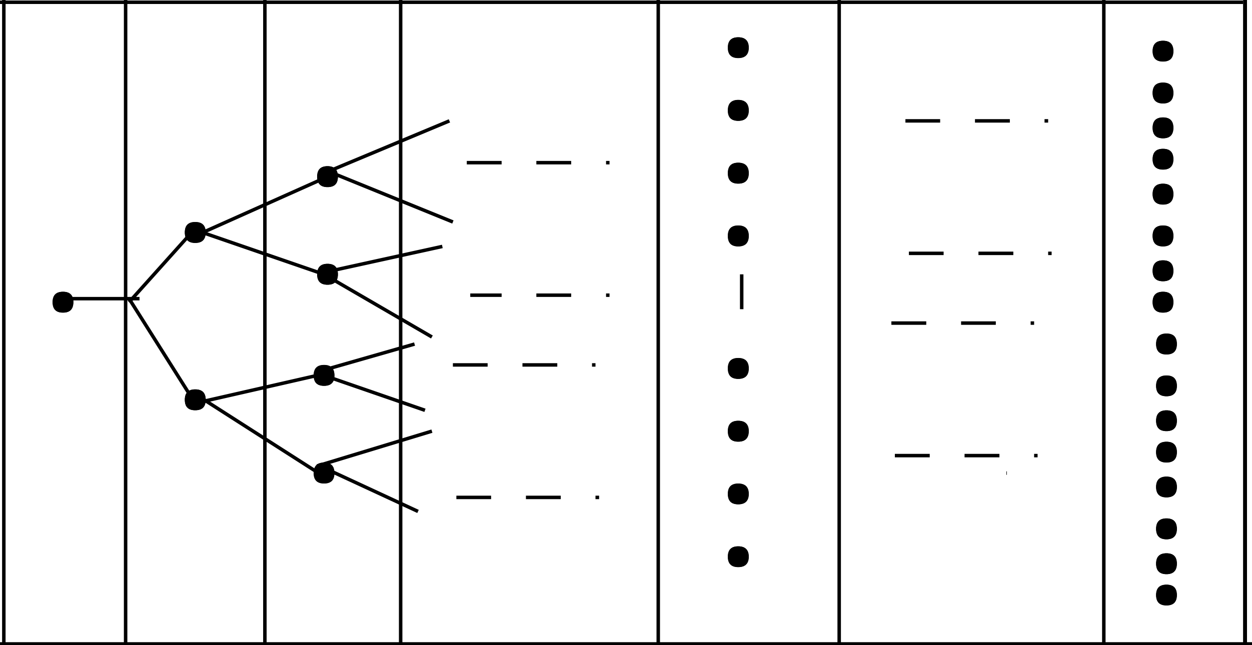
When does a cascade end?

- Remember:

- Cascade ceases when knock-on energy is:

Gener-ation	0	1	2		N		final
average energy	E	E/2	E/4	…………………	$E/2^N$	…………………	$2E_d$
Number displaced	1	2	4	…………………	2^N	…………………	ν



K-P Model

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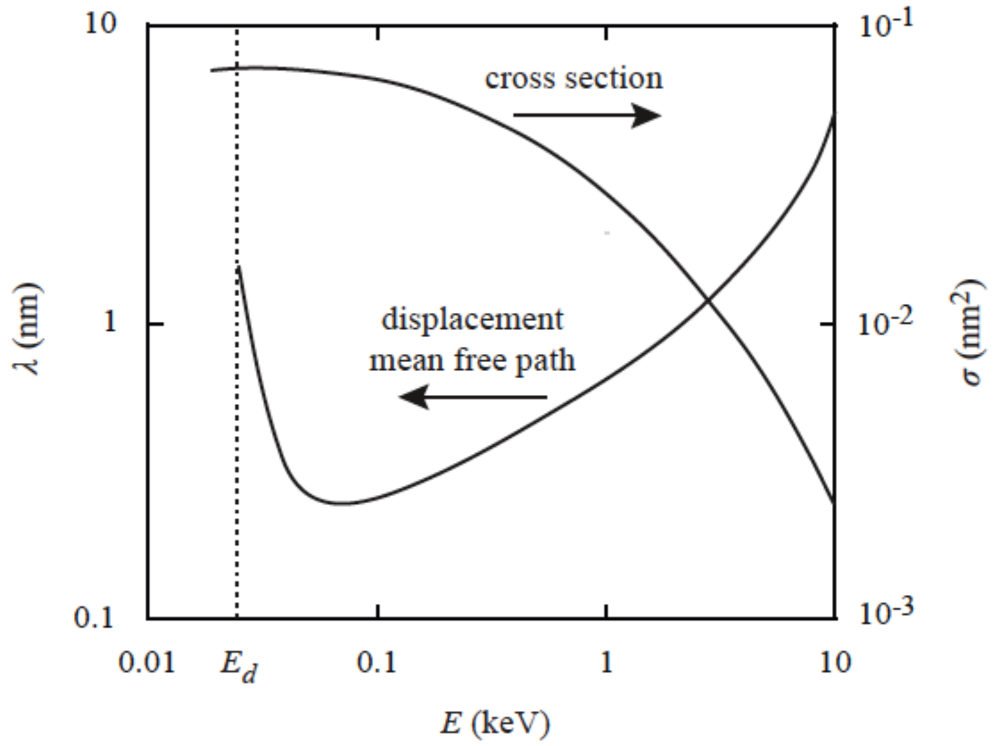
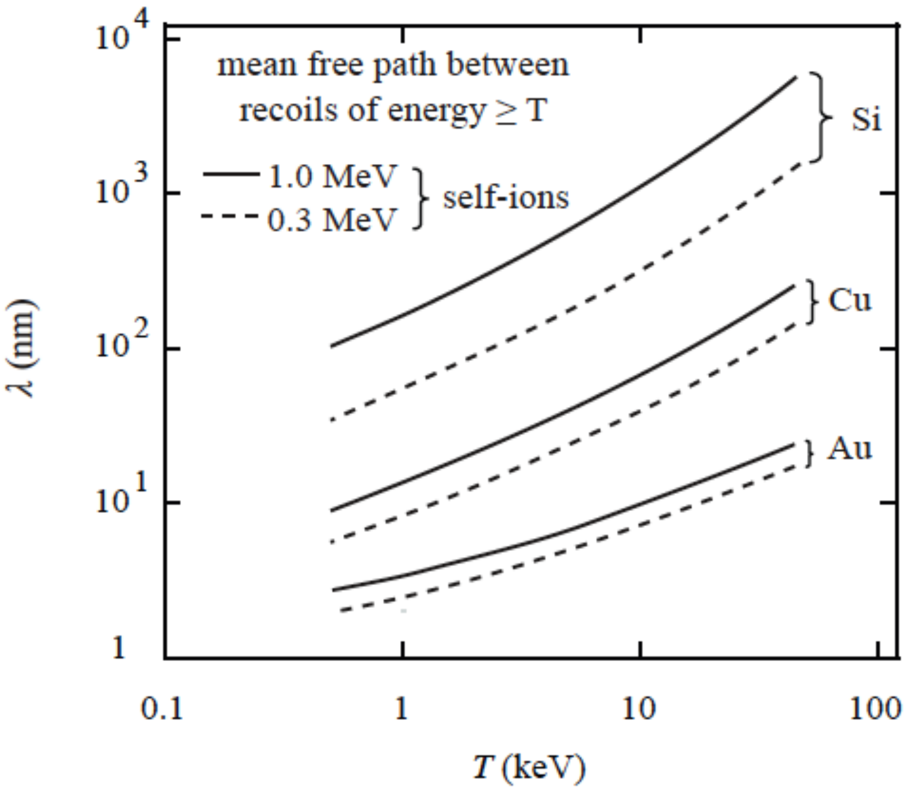
Mean free path between recoils

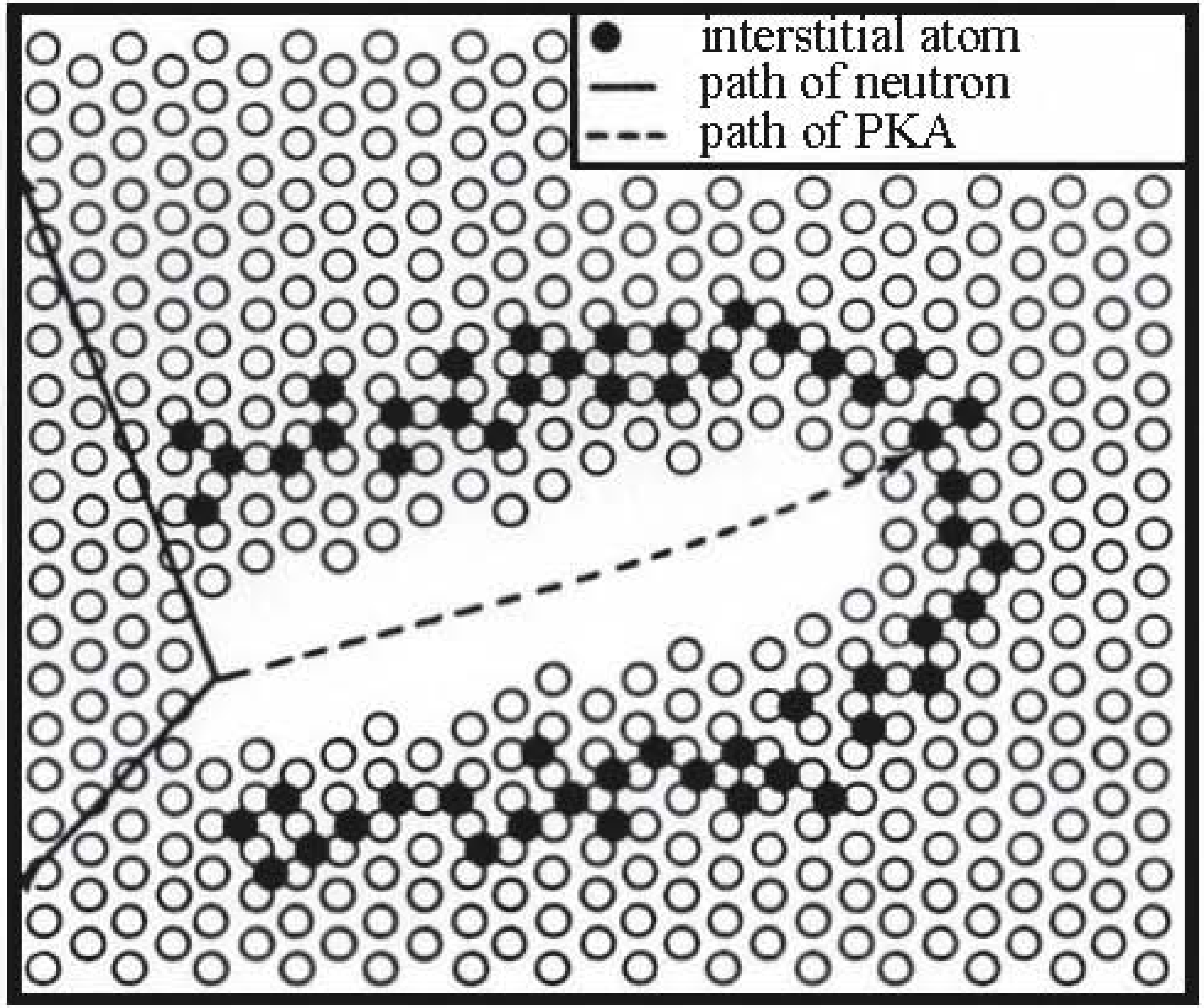
- Brinkman calculated the mean free path, determined spacing approached atomic separation distances.
  - Led to the realization that many cascades are not a collection of isolated Frenkel pairs



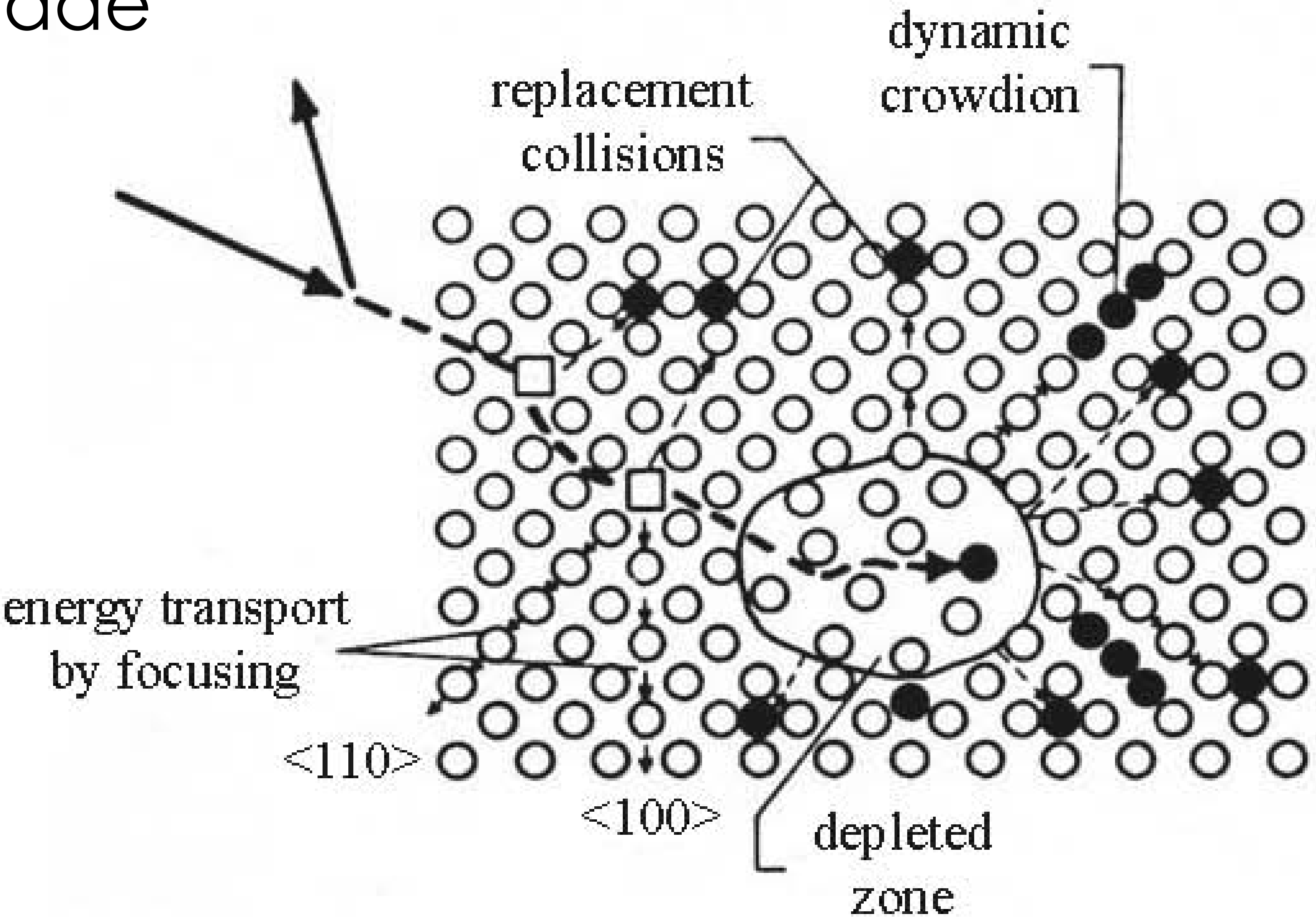


Original conception of the damage cascade

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



Another revised conception of the damage cascade



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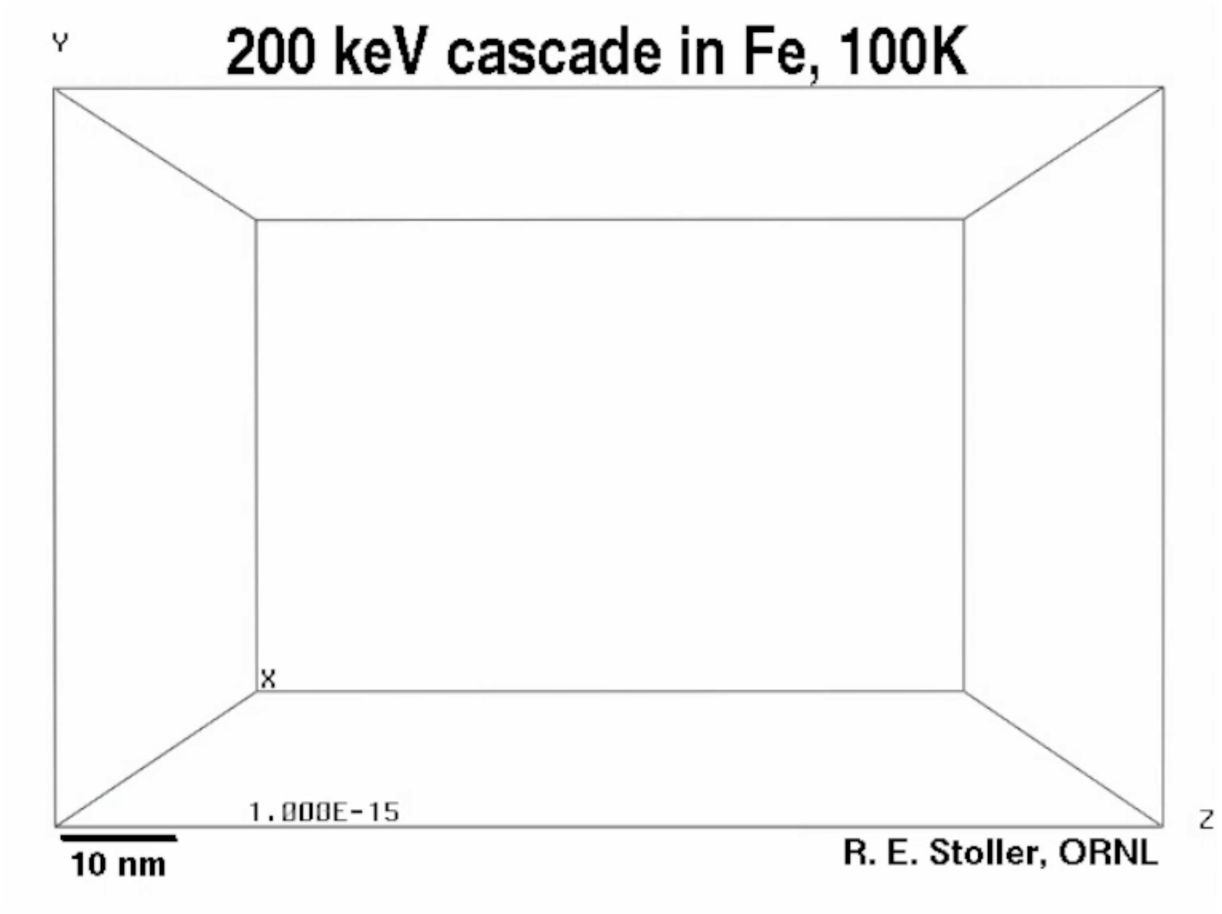
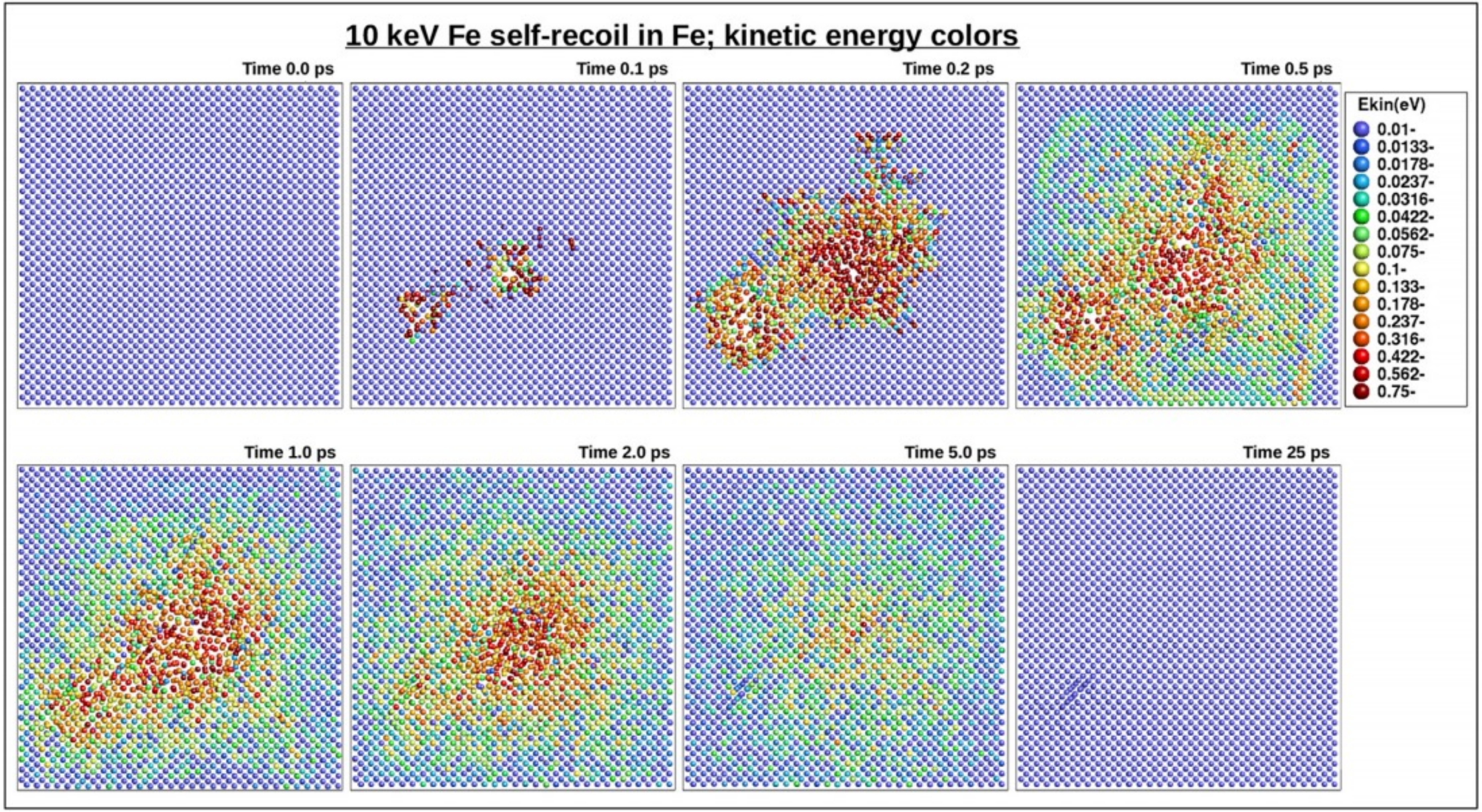
A more realistic visual:

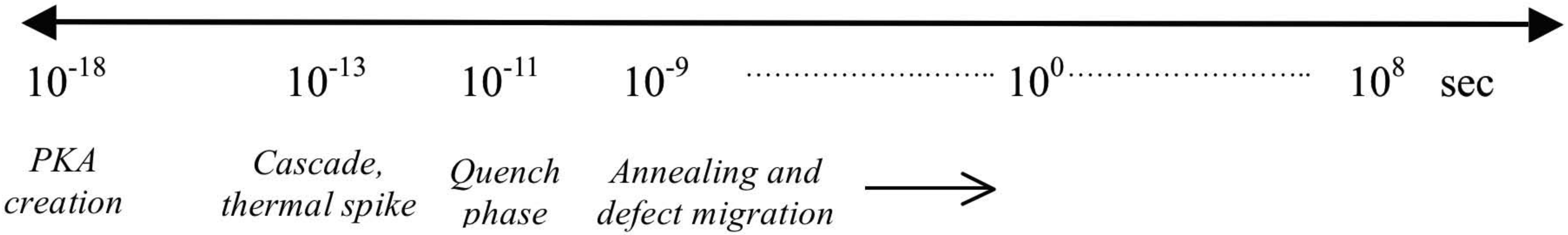
3.1 Molecular Dynamics (MD) simulation of the development of a cascade from a 20 keV recoil in iron at 100K. Note the striking difference in defect density between the peak of the ballistic regime (~1 ps) and that at the end of the quench (~5 ps). (courtesy, R. Stoller, Oak Ridge National Laboratory)



Visual snapshot of a cascade and stages

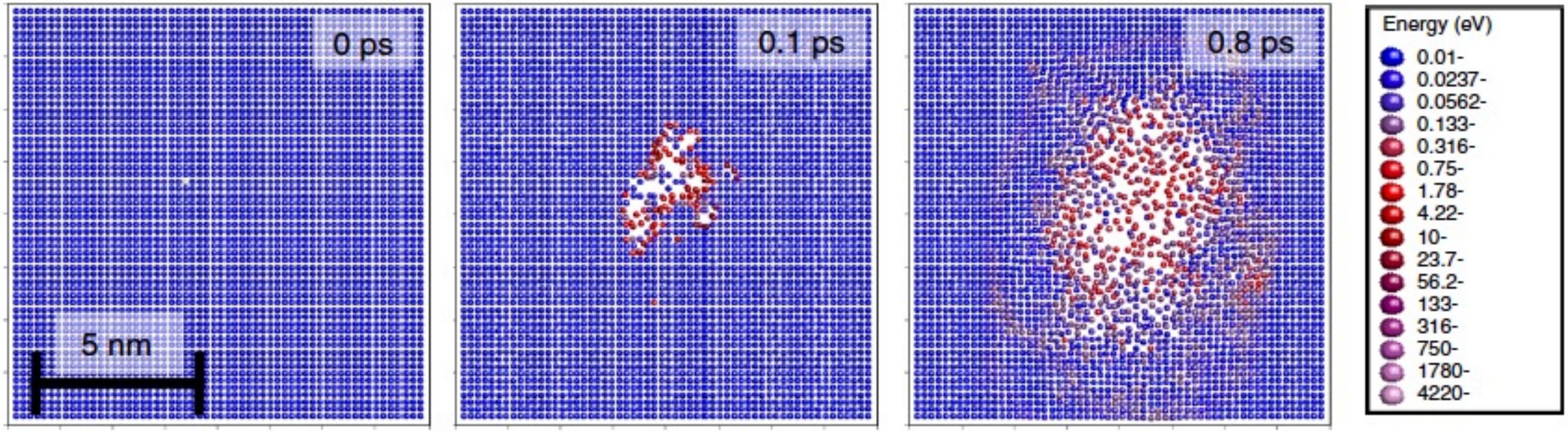


Cascades have four distinct stages:



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)

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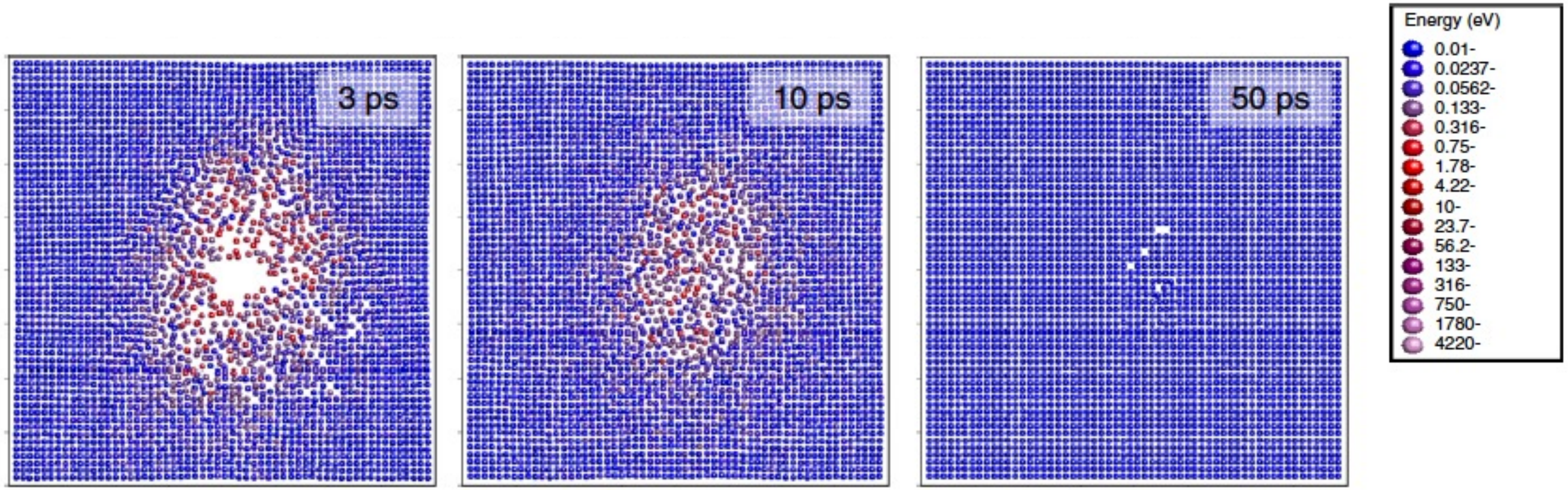
Quenching -> Annealing



- 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

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Quenching -> Annealing

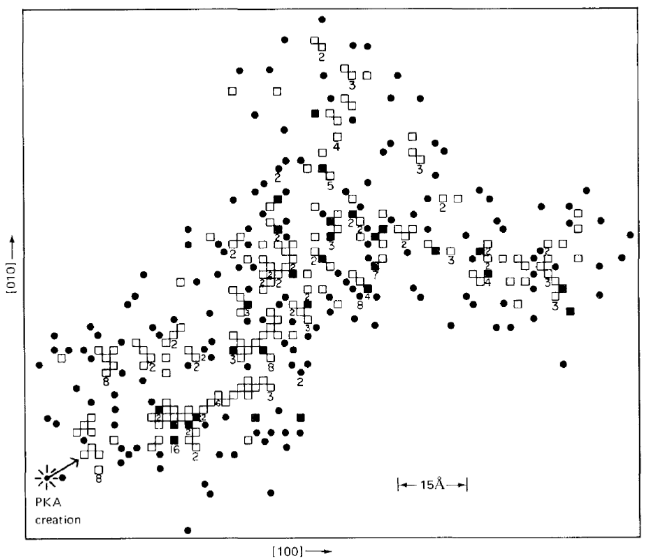

Fig. 17.27 Displacement spike due to a 20-keV PKA in iron projected onto the (001) plane (0°K). [After J. R. Beeler, Jr., *Phys. Rev.*, 150: 470 (1966).]

800k anneal

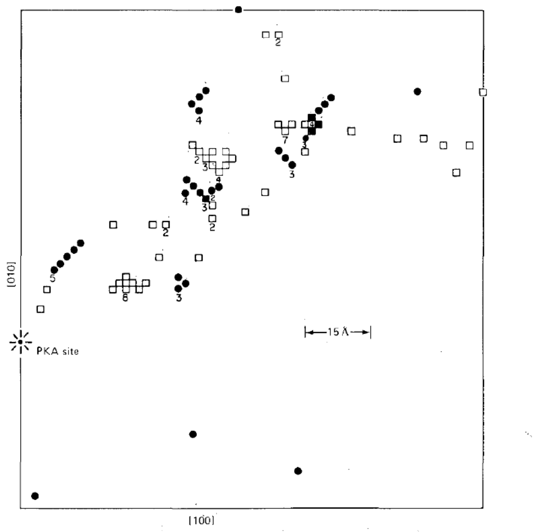

Fig. 17.28 Displacement spike [projected onto the (001) plane] due to a 20-keV PKA in iron after annealing at 800°K (6000 interstitial jumps and 60 vacancy jumps). The preannealed spike is shown in Fig. 17.27. Numbers on the diagram denote cluster sizes. Twelve interstitials have migrated outside the 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

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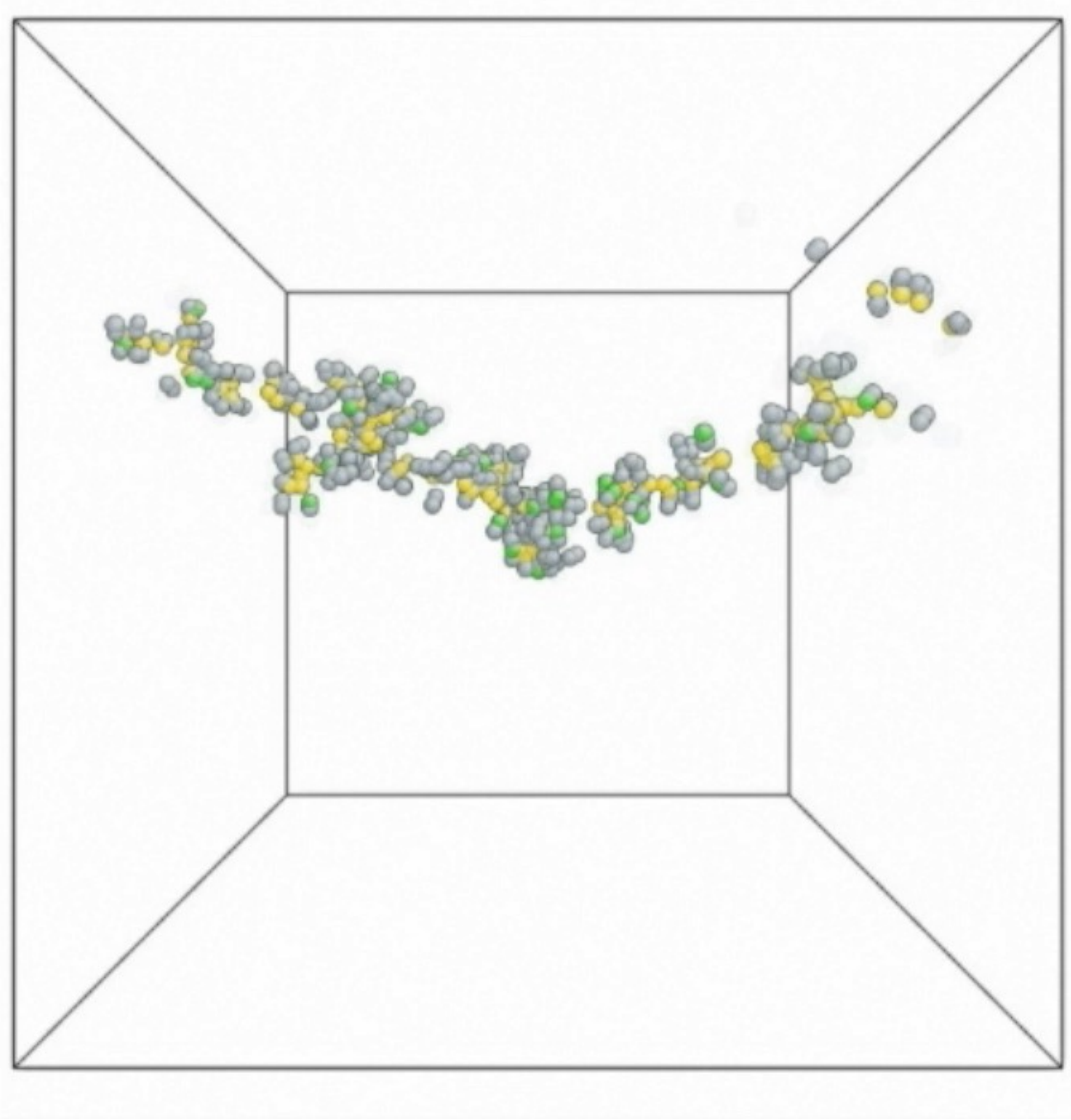
A more realistic visual:

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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MILK PRODUCTION UPDATE - JULY 2022

JULY 2022 Current Month Production
Top 6 States

Million lbs.		% change vs. year ago	+/- MM lbs. vs. year ago	Current Share
California	3,515	+2.2%	+77	18.4%
Wisconsin	2,722	-0.3%	-7	14.2%
Idaho	1,453	+1.5%	+21	7.6%
Texas	1,381	+6.0%	+78	7.2%
New York	1,336	0.0%	+0	7.0%
Michigan	993	-3.8%	-39	5.2%
Total US: 19,140MM lbs.		+0.2%	+43	100.0%

JAN-JUL 2022 Year-to-Date Production
Top 6 States

Million lbs.		% change vs. year ago	+/- MM lbs. vs. year ago	Current Share
California	24,843	-0.3%	-71	18.6%
Wisconsin	18,613	+0.3%	+48	14.0%
Idaho	9,678	+0.4%	+41	7.3%
Texas	9,650	+5.4%	+493	7.2%
New York	9,129	-0.4%	-40	6.9%
Michigan	6,854	-3.1%	-217	5.1%
Total US: 133,258MM lbs.		-0.6%	-833	100.0%

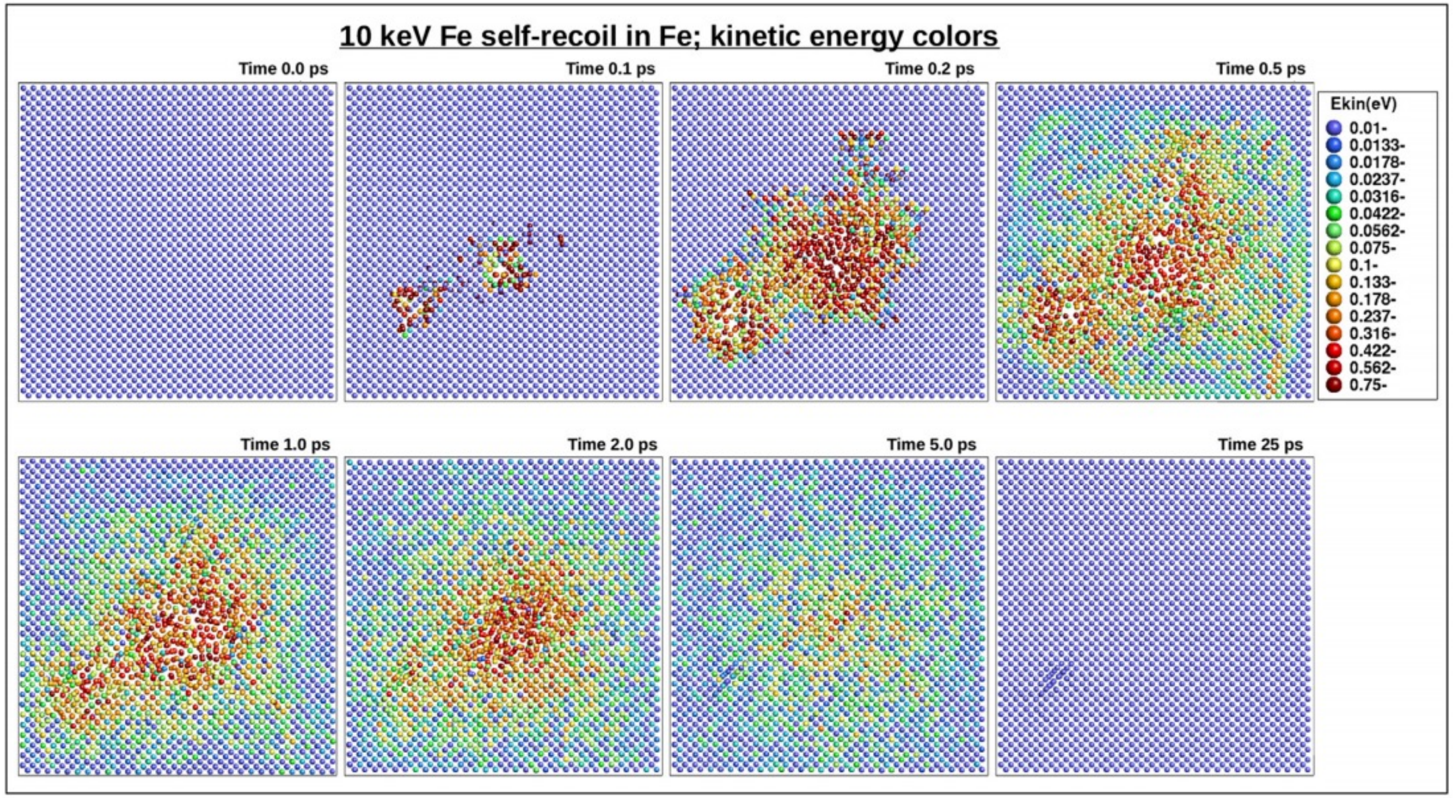
	WISCONSIN	CALIFORNIA	TOTAL U.S.
			
Number of Cows	1.272MM -0.5% vs. Jul'21	1.723MM +0.2% vs. Jul'21	9.416MM -0.7% vs. Jul'21
Milk per Cow	2,140 lbs. +0.2% vs. Jul'21	2,040 lbs. +2.0% vs. Jul'21	2,033 lbs. +0.9% vs. Jul'21
Total Milk Production	2,722MM lbs. -0.3% vs. Jul'21	3,515MM lbs. +2.2% vs. Jul'21	19,140MM lbs. +0.2% vs. Jul'21

DAIRY FARMERS OF WISCONSIN®

Source: USDA/NASS, Milk Production

According to one website, the what percent of the annual dairy cow milk supply is used in Wisconsin to make cheese?

Visual snapshot of a cascade and stages



- General result:
  - Isolated interstitials or interstitial-pairs outside the thermal spike region
  - Vacancies randomly distributed
  - "Core" of vacancy cluster in the center of the thermal spike

https://www.nature.com/articles/s41467-018-03415-5

Cascade Overlap

- Cascades occurring one-after another in the same region or those close to each other can impact surviving defects
  - What happens depends on many factors including PKA direction and separation
- Vacancy core can be destroyed by lon-range interstitial mobility from nearby collision cascade

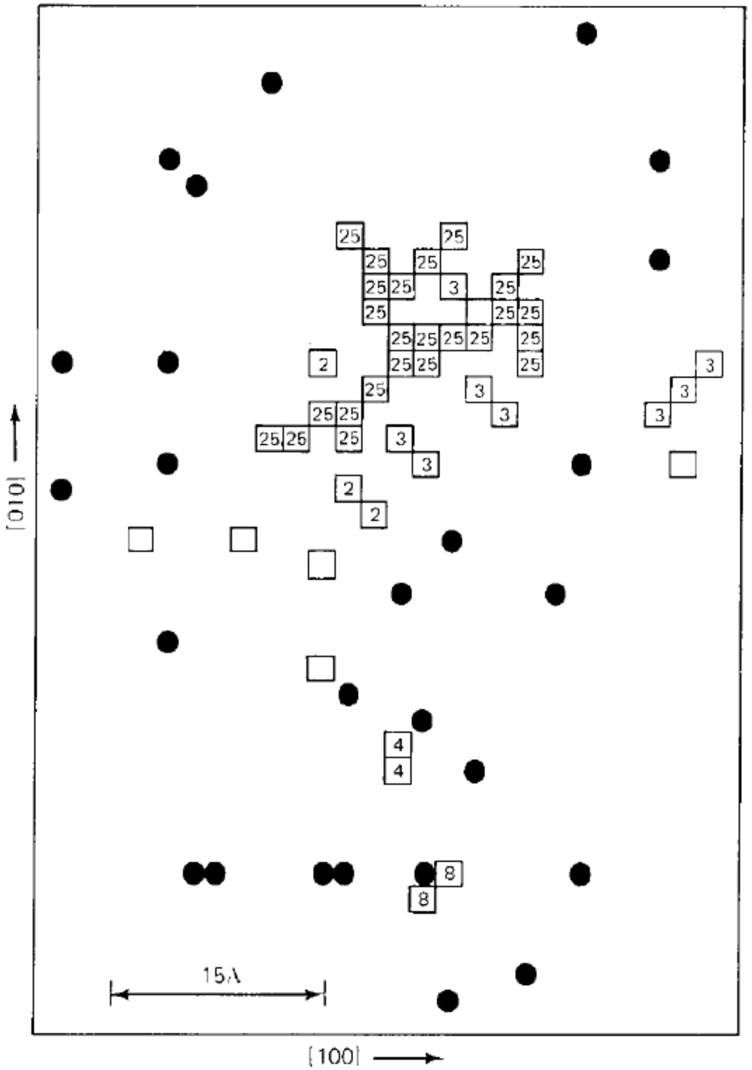


Fig. 17.30 A 25-vacancy cluster formed by the overlap of three successive 5-keV displacement spikes in copper (0°K). (After Ref. 30.)

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Different radiation produces different cascades

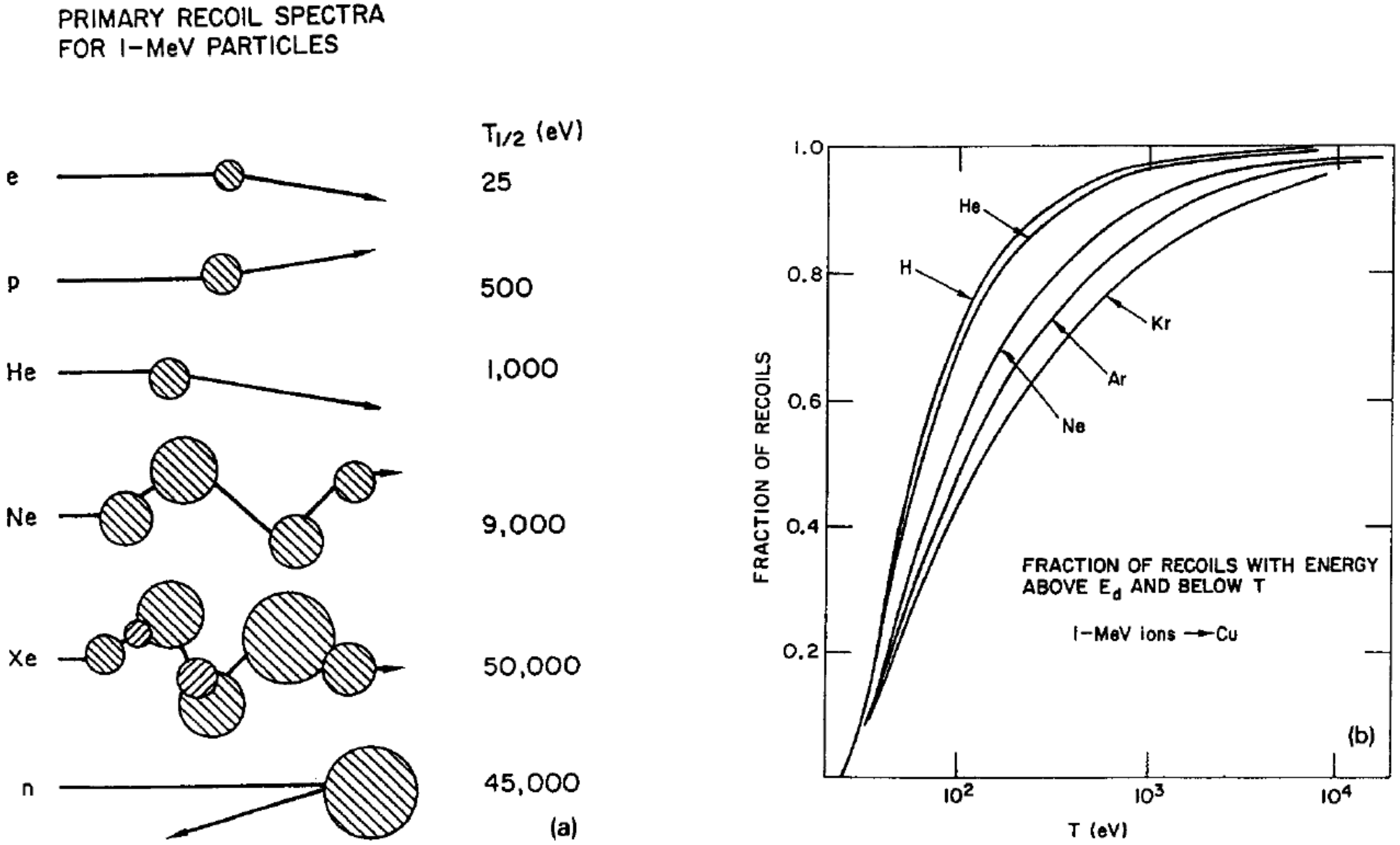

Fig. 2. (a) Qualitative representation of the primary recoil spectra for 1 MeV particles in Cu. Circles indicate where energetic recoils occur and their size indicates the amount of energy transferred to the recoil atom. $T_{1/2}$ refers to a "typical" recoil energy which is defined below. (b) Integral primary recoil spectra for 1 MeV particles in Cu. It is the integral fraction of primary recoils between the threshold energy and energy, T.

https://doi.org/10.1016/0022-3115(94)90006-X

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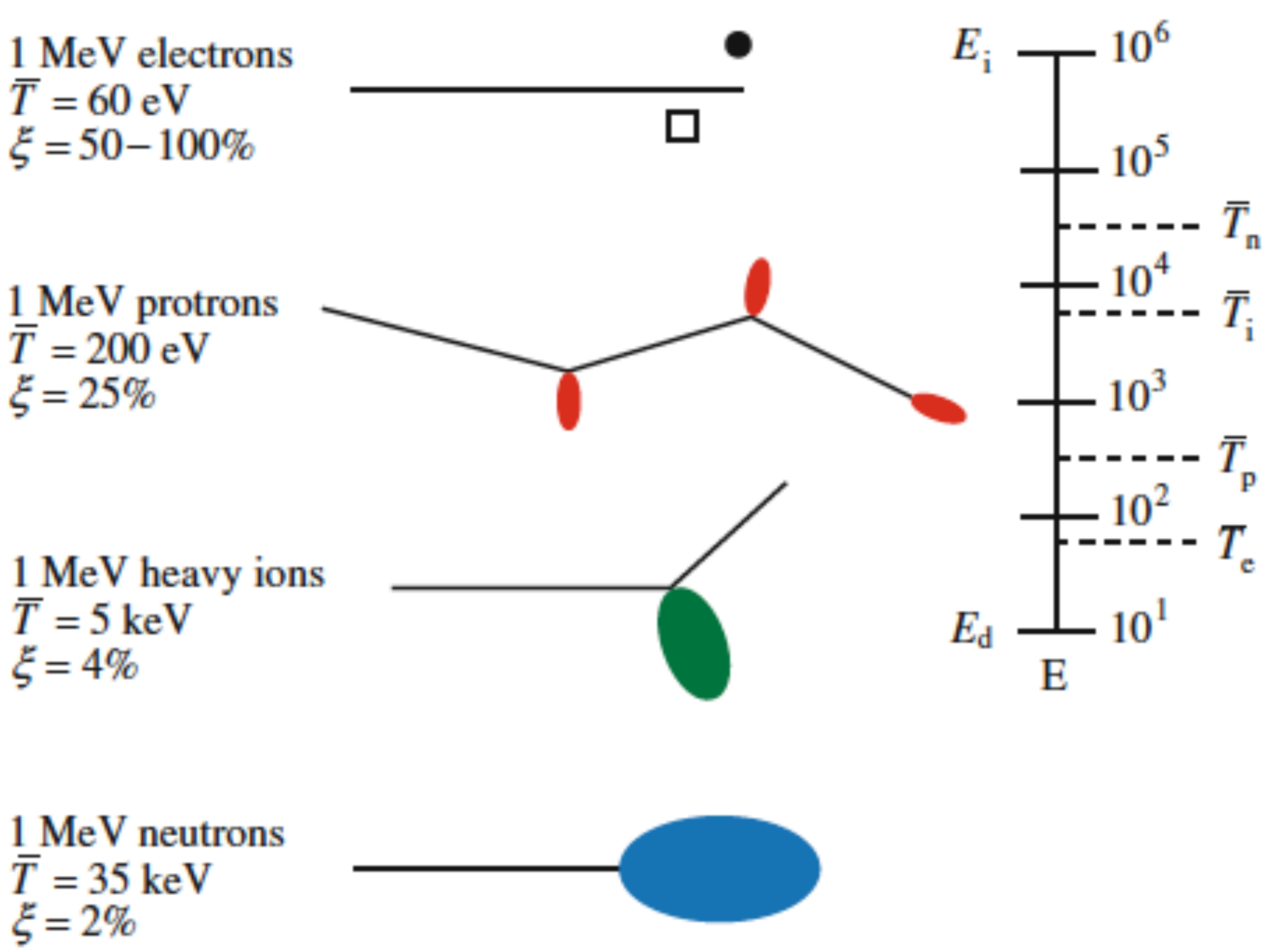
Different radiation produces different cascades

<u>Mass & Charge:</u>

Increasing mass, same charge

Moderate mass, no charge



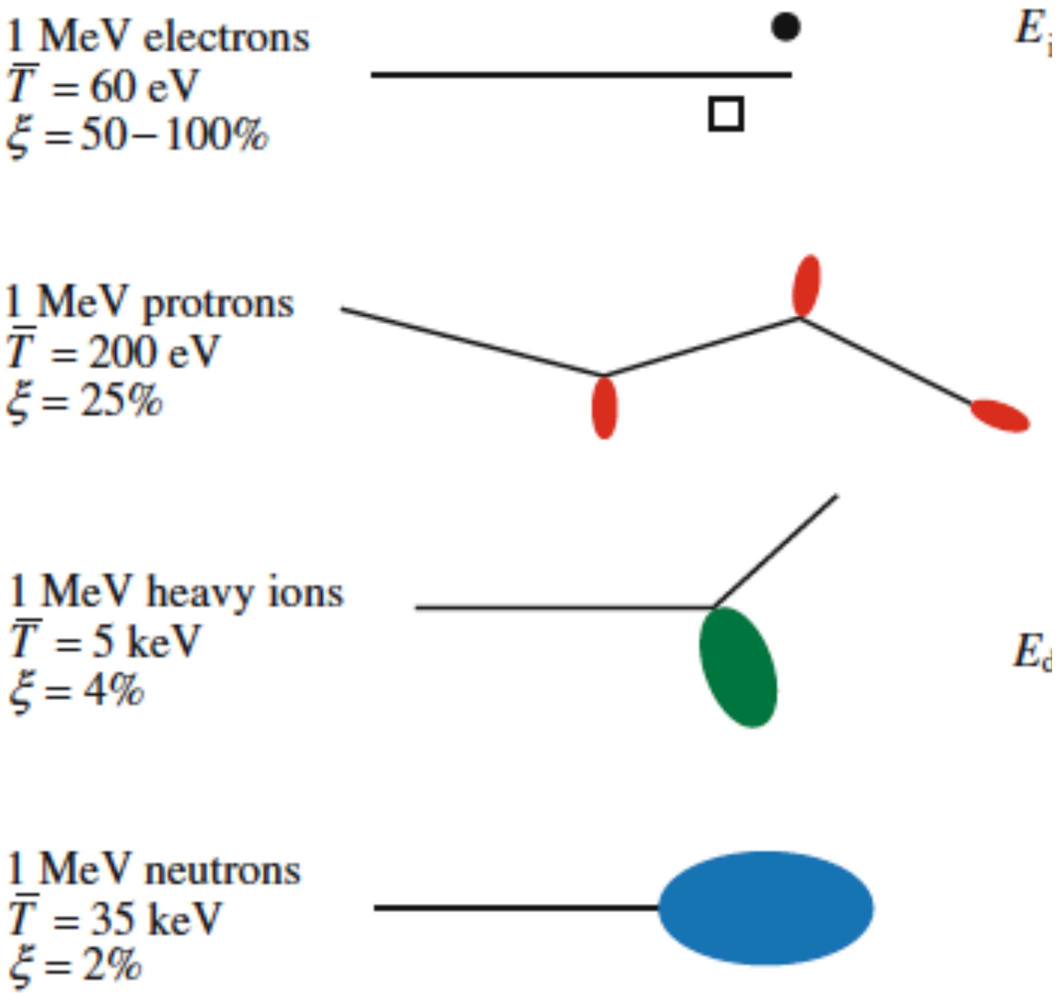
<u>Stopping mechanism:</u>

Displacement Efficiency

- The displacement efficiency ξ, is the fraction of the “ballistically” produced Frenkel pairs (NRT dpa) that survives the cascade quench.

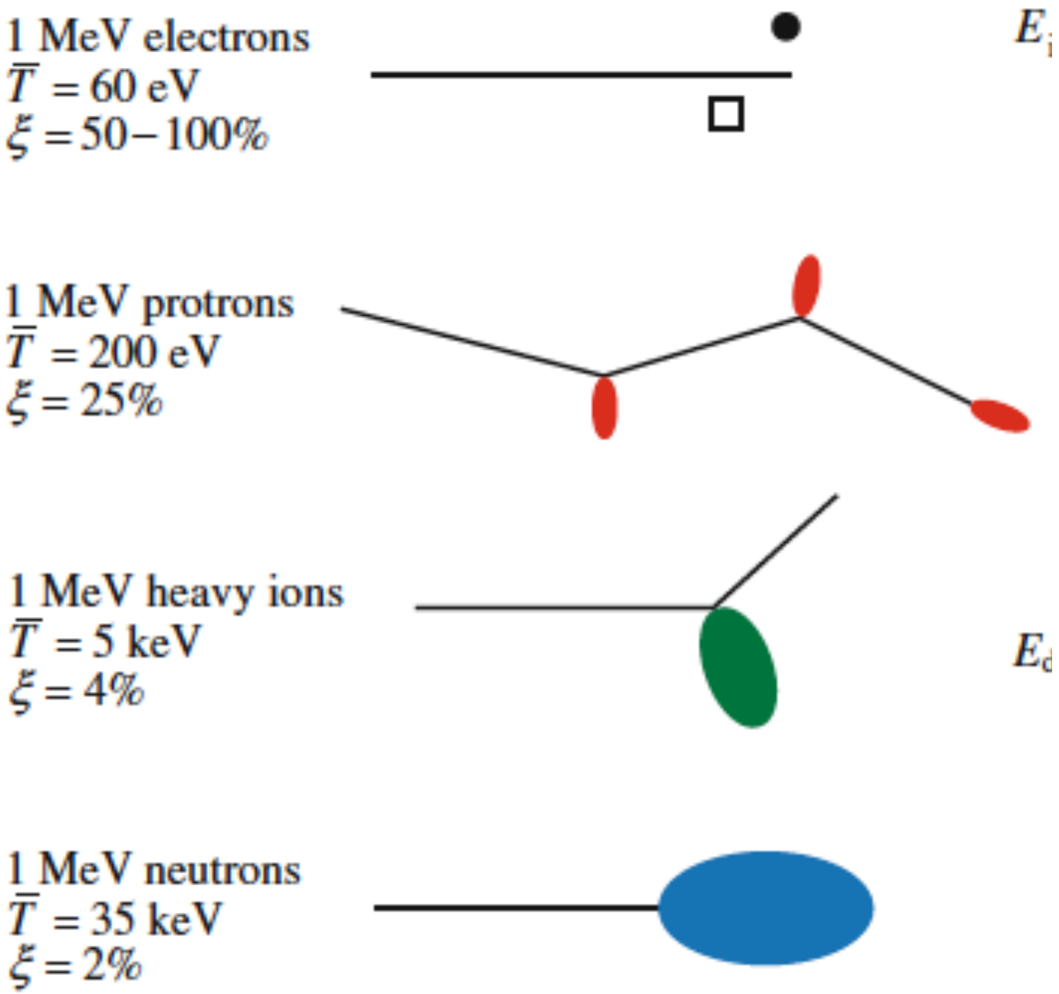
$$\xi = \delta_i + \eta_i + \eta_i = \delta_v + \eta_v + \eta_v$$

$\eta_{i,v}$ = isolated point defect fraction
$\delta_{i,v}$ = clustered fraction including mobile defect clusters
ς = fraction initially in isolated or clustered form after the cascade quench that is annihilated during subsequent short term (> 10^{-11} s) intracascade thermal diffusion



Displacement Efficiency

- What does this mean if we want to emulate neutrons with ions?



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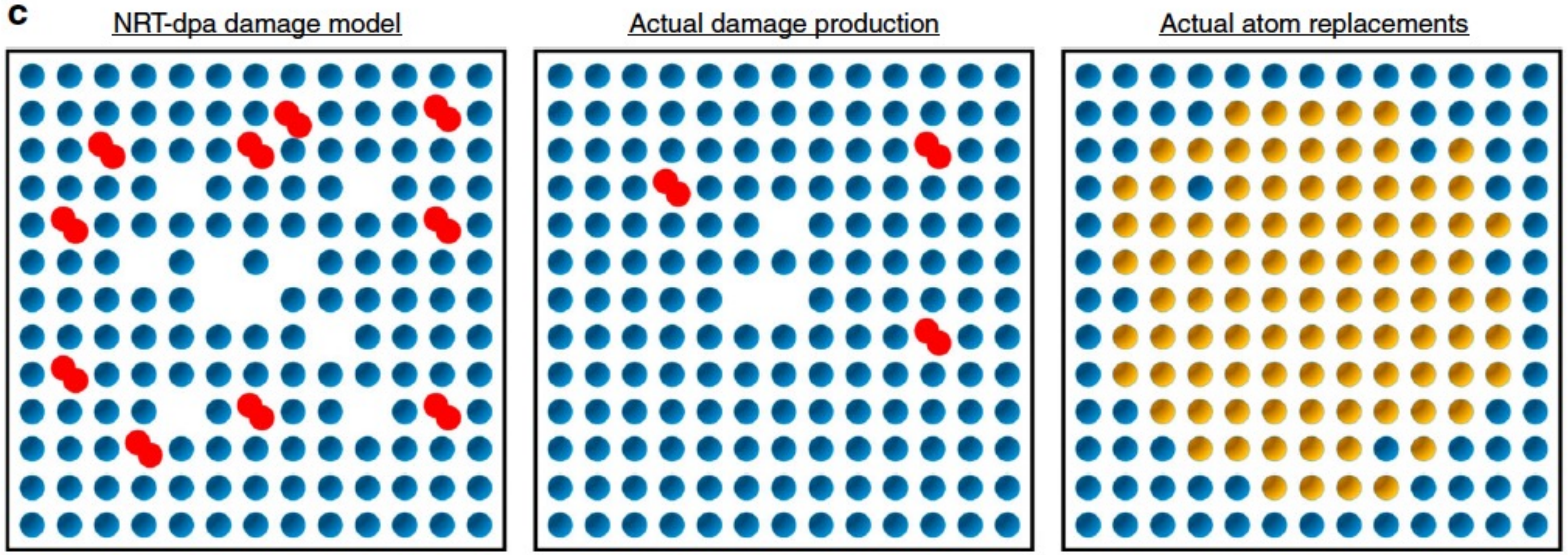
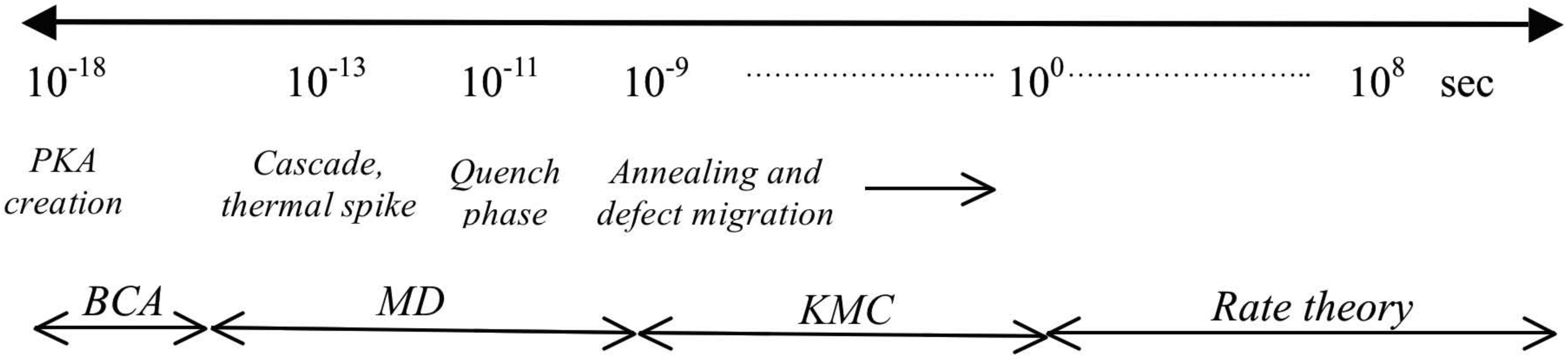
Modification to NRT model based on cascade physics



<u>Arc-dpa: Athermal recombination corrected dpa</u>
- Accounts for enhanced recombination in metals in a cascade

<u>Rpa: Replacements per atom</u>
- Provides a measure of the volume of irradiated material directly affected by the cascade
  - Implications on phase stability and mixing

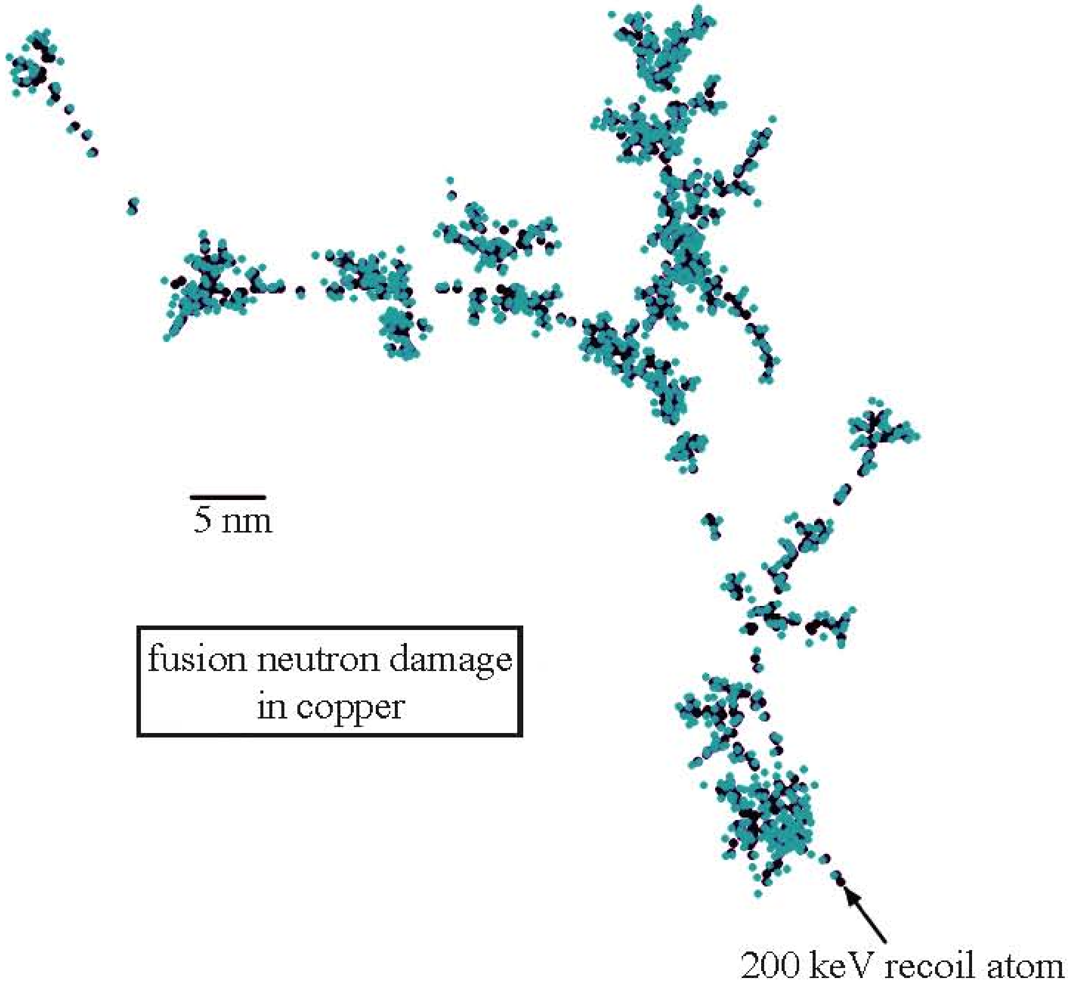
Cascades have four distinct stages:



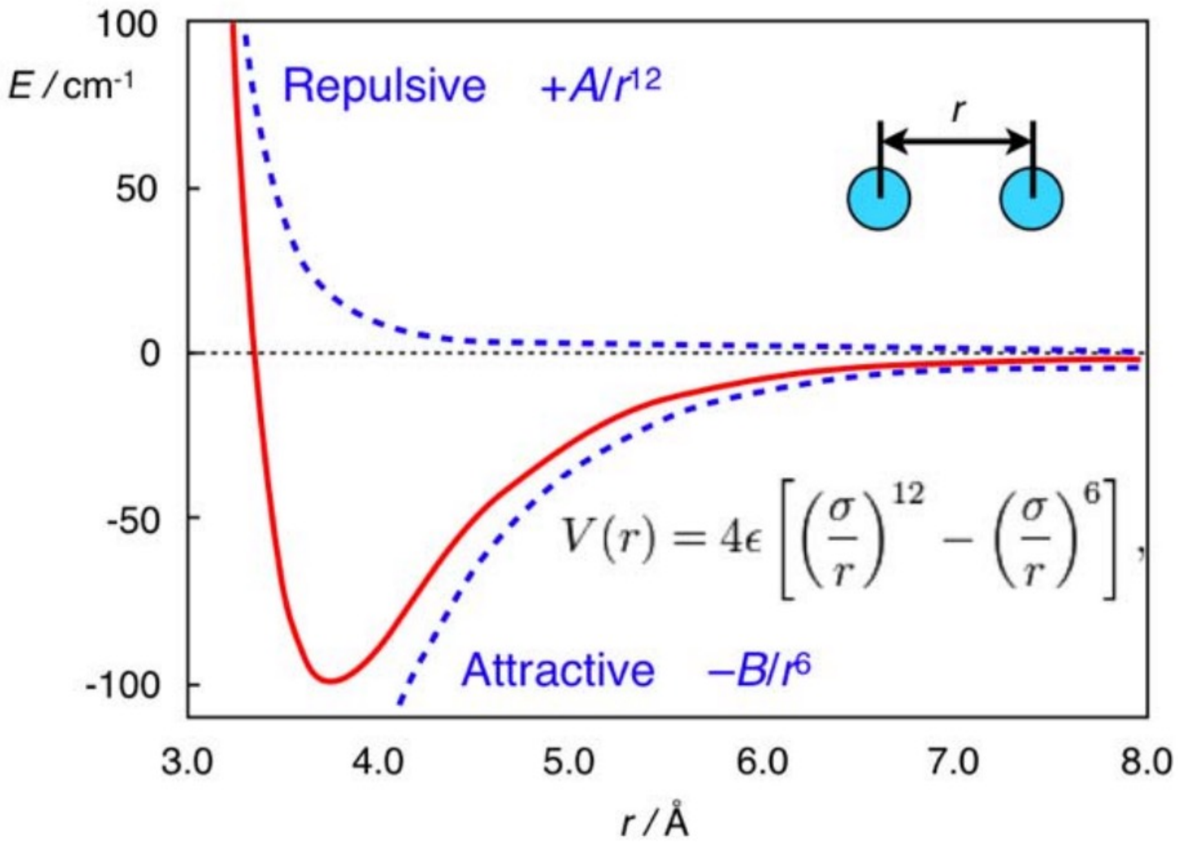
1. Collisional
2. Thermal spike
3. Quenching
4. Annealing

Simulation methods - Binary Collision Approx.:

- Binary Collision Approximation:
  - Uses interatomic potentials to allow atoms to move
  - Does not restrict crystallinity
  - Reasonable for collision cascades



Simulation methods – Molecular Dynamics



- Lennard-Jones potentials are widely used
- LAMMPS software package widely used

- Solve F= ma for every pair of atoms
- Interatomic potentials are the key to interactions

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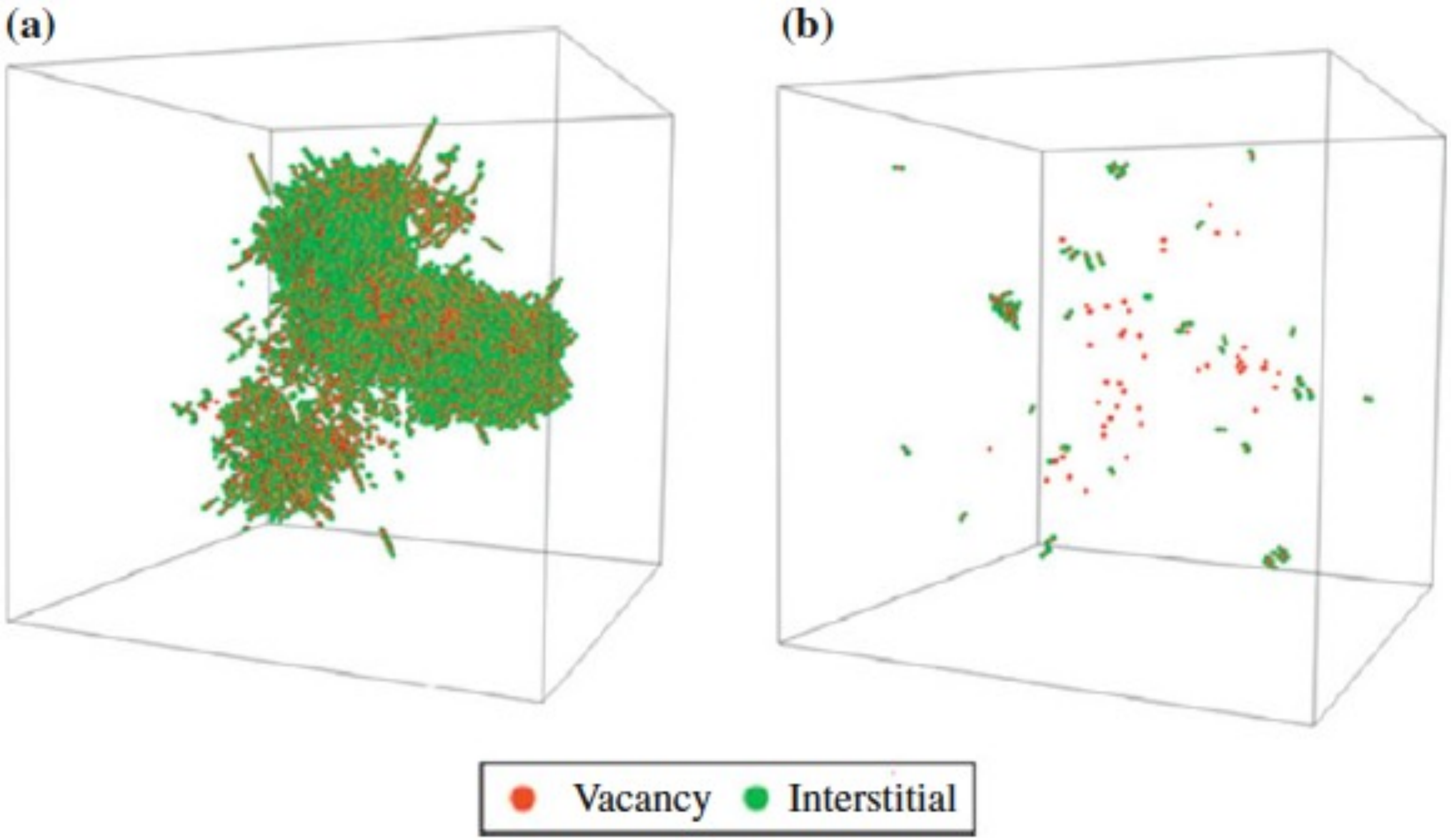
Simulation methods – Molecular Dynamics



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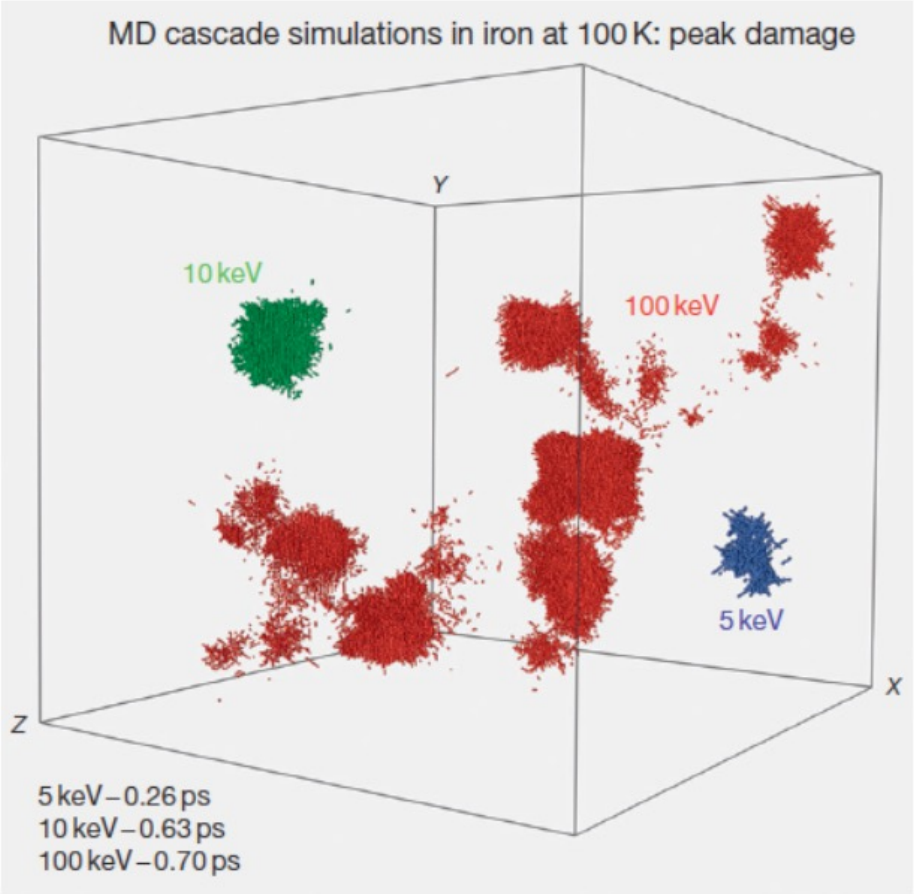
Simulation methods – Molecular Dynamics



- Solve F= ma for every pair of atoms
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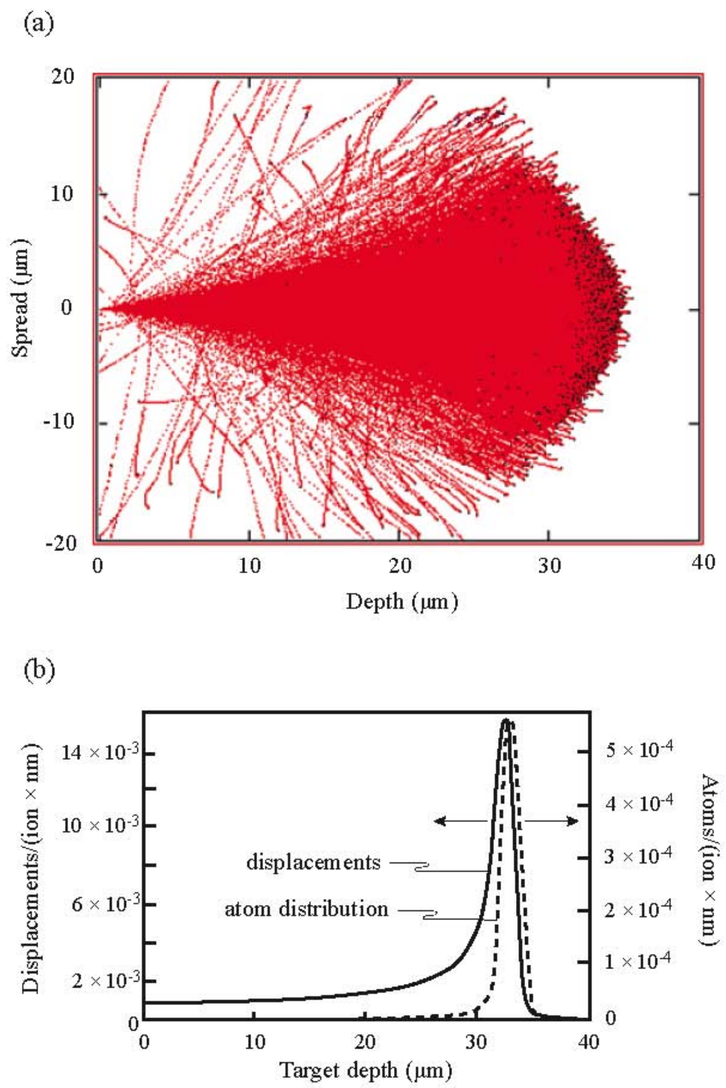
Simulation methods – Monte Carlo

SRIM is the most widely used simulation for damage of ions and uses a Monte Carlo approach

- Takes into account:
  - Material composition
  - Material configuration (e.g. layers)
  - Displacement energy of each element in each layer
  - Density
  - Incident ion type & energy
  - Type of calculation

Debated in literature!



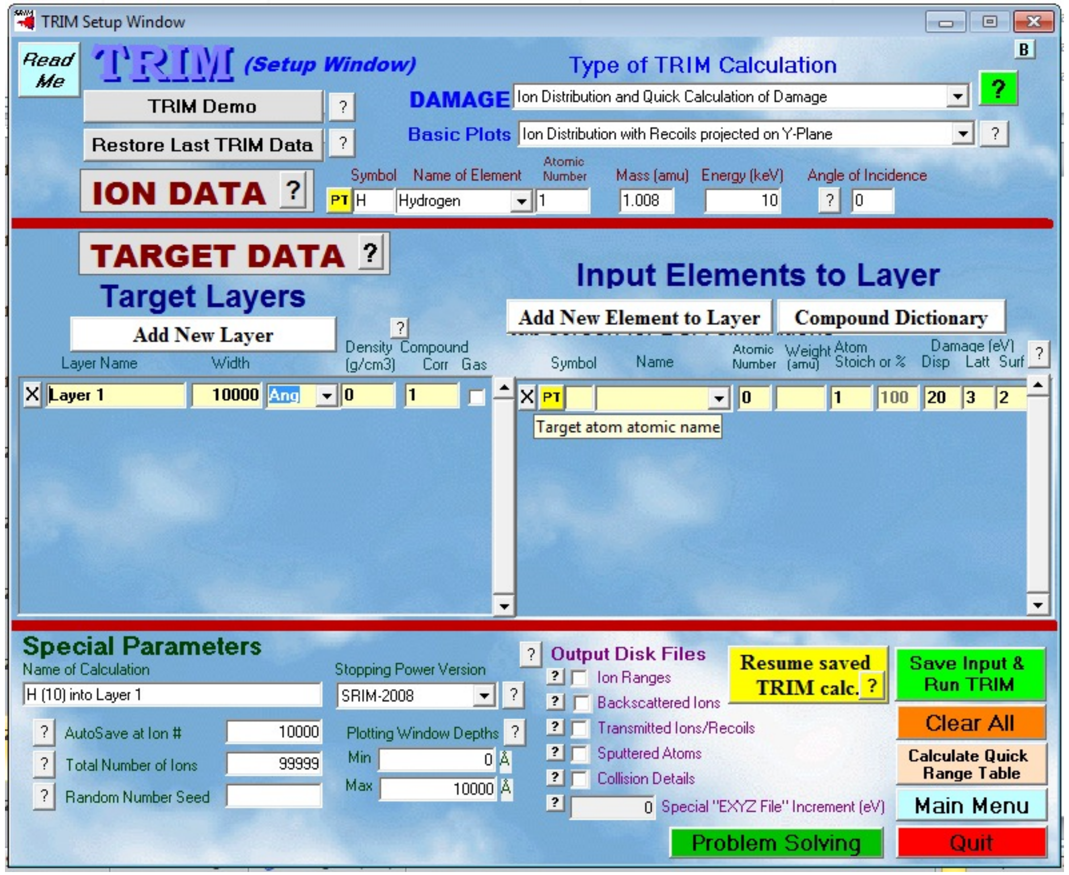
The SRIM software

The SRIM software is freely available at the SRIM web pages

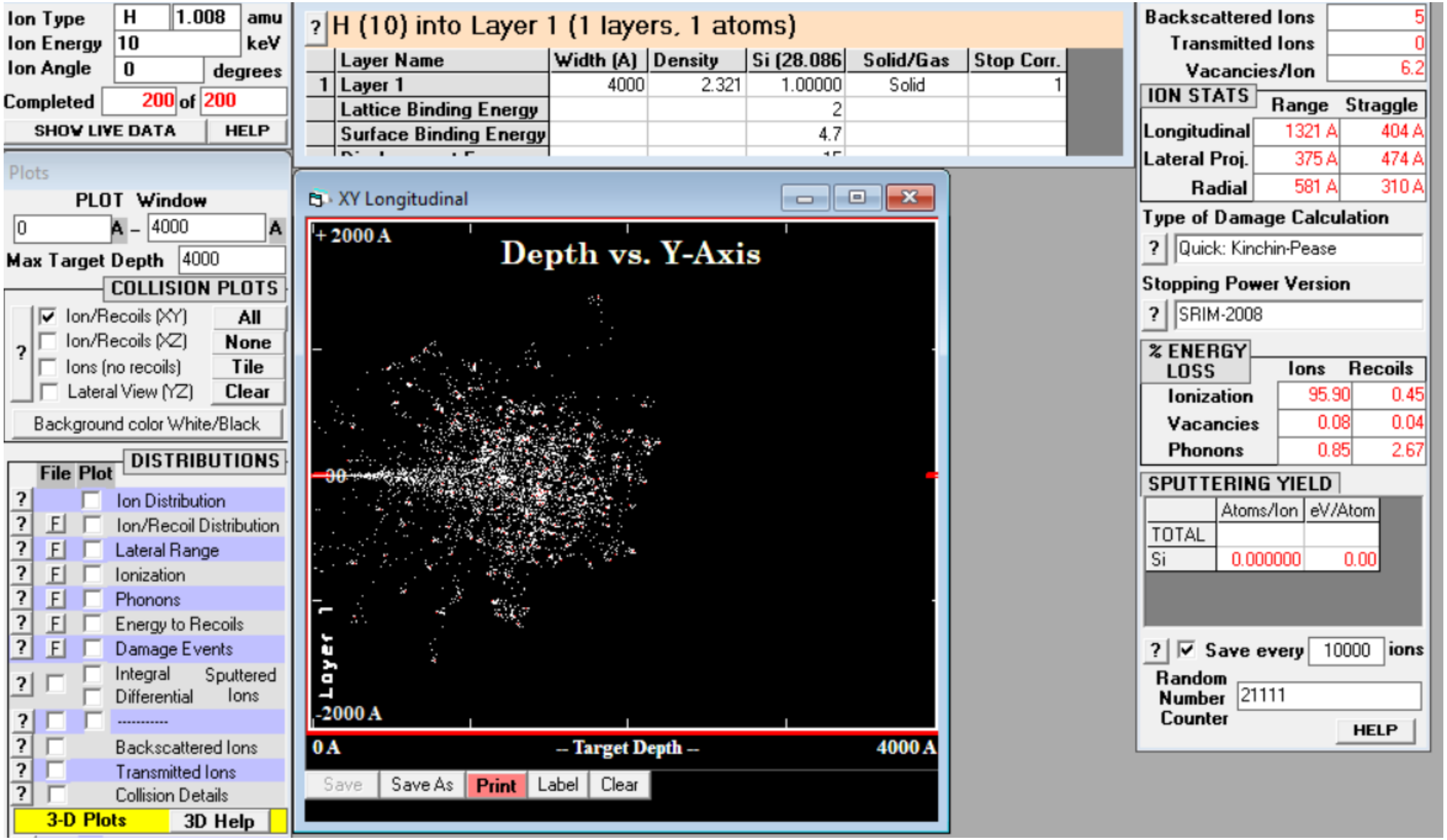
- Often also called TRIM due to the earlier name "Transport and Range of Ions in Matter"

- It can calculate any stopping power (electronic or nuclear) in any material, including compounds and multilayer one
- Includes electronic stopping in all calculations
- Downsides:
  - Only amorphous materials modelled => no channeling
  - No temperature dependence
  - It only works on Windows computers, is not open source , and is programmed in a quite old fashioned way with Visual Basic
  - Because of this, installing it on modern Windows is a hassle
  - Tip: for it to work at all, one needs to set Regional settings to US English in Windows…

The SRIM software



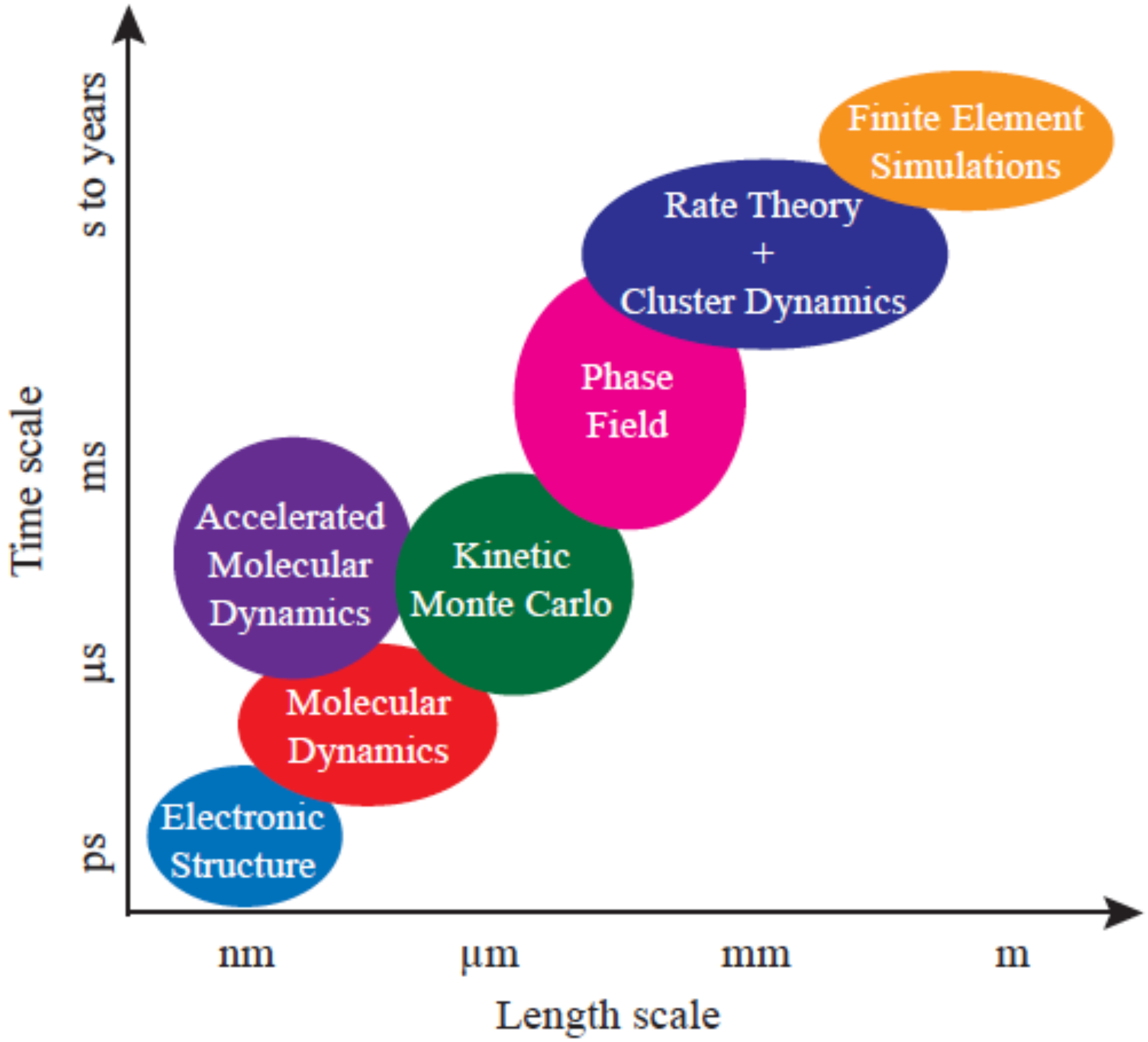
The SRIM software



SRIM notes

- SRIM can be somewhat speeded up by closing all the output windows, and can be well ran in the background on modern multi core processors
- Several output options exist: ion ranges, nuclear and electronic deposited energy, sputtering yield
- For detailed analyses output of file COLLISON.DAT outputs data on all ions and recoils created during the whole simulation
- Do not use SRIM blindly: there are major caveats and pitfalls in using it, and not knowing them can lead to too much trust in accuracy of results or even outright wrong physics

Time/length scales of various computational techniques



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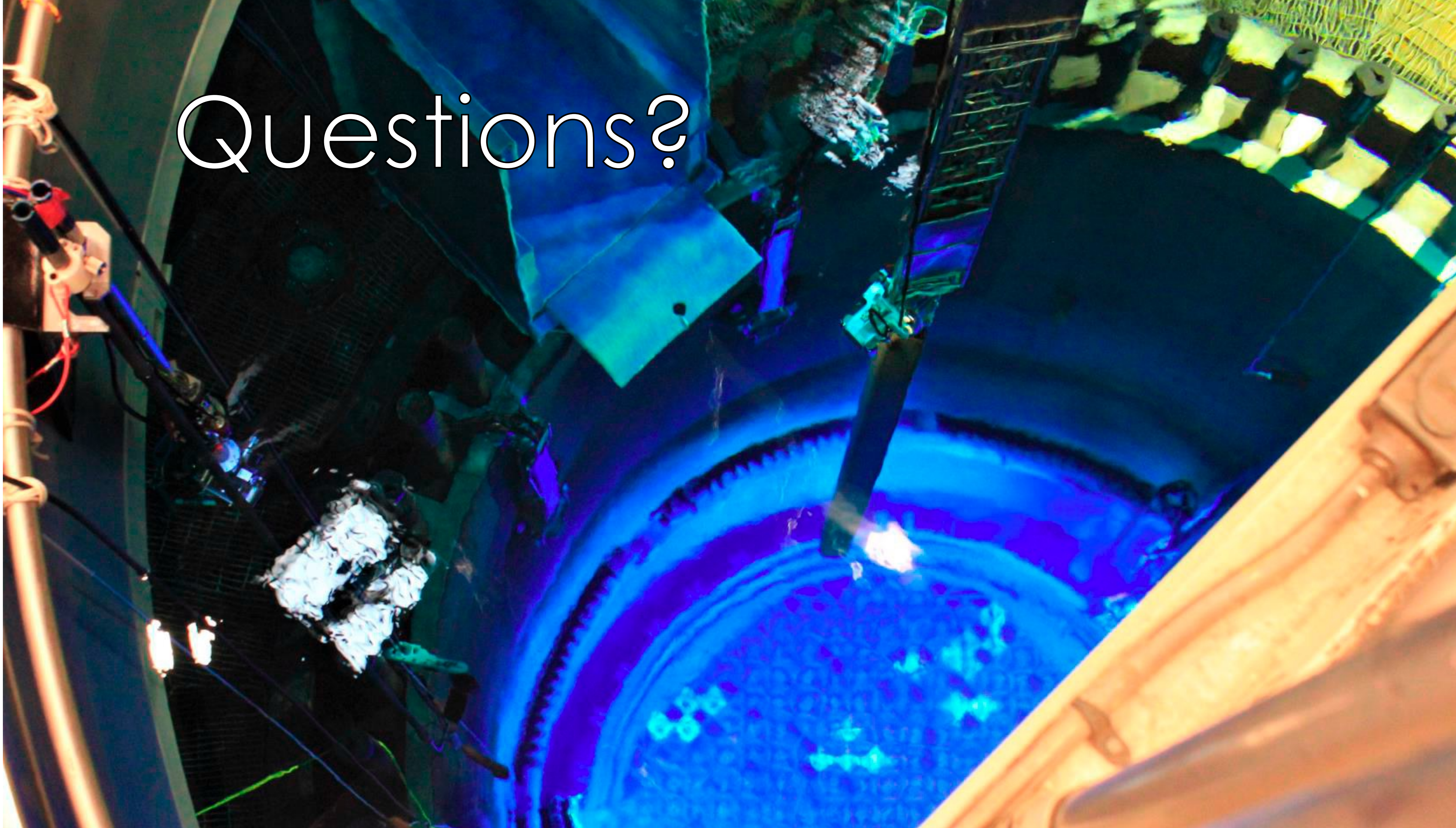
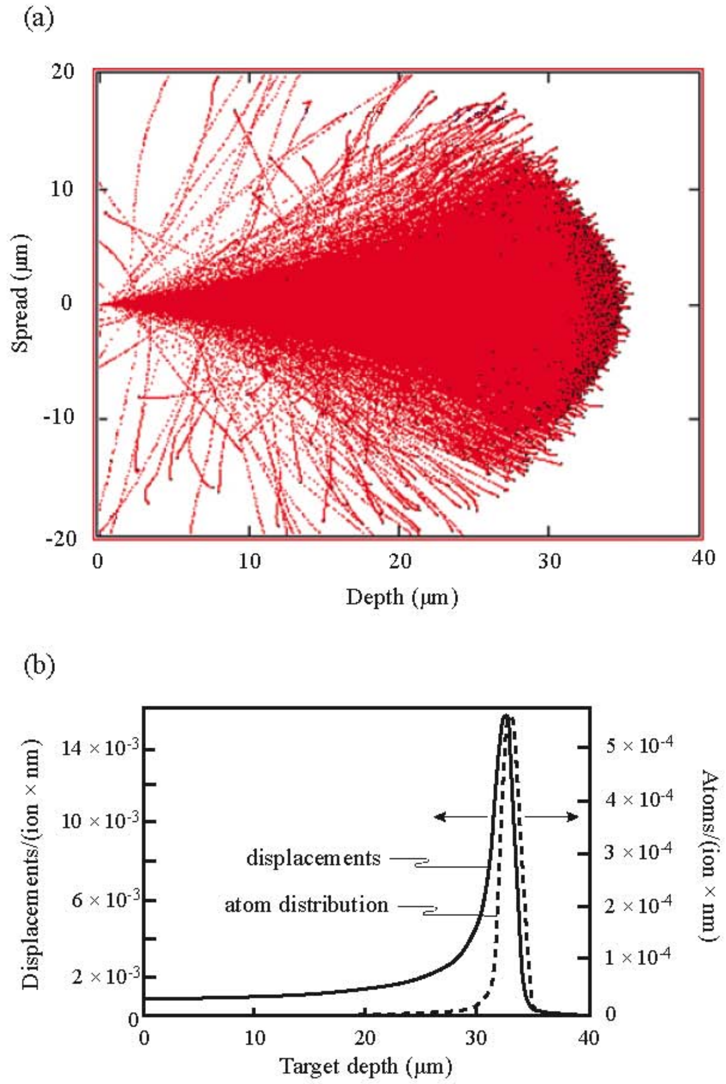
Questions?



Simulation methods – Monte Carlo

SRIM is the most widely used simulation for damage of ions and uses a Monte Carlo approach

- Limitations:
  - No time dependence – you aren't seeing the effects of does rate (more later in lecture series)
  - No temperature dependence
  - No crystal structure



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