

Damage Cascade

K.G. Field^{1,a},

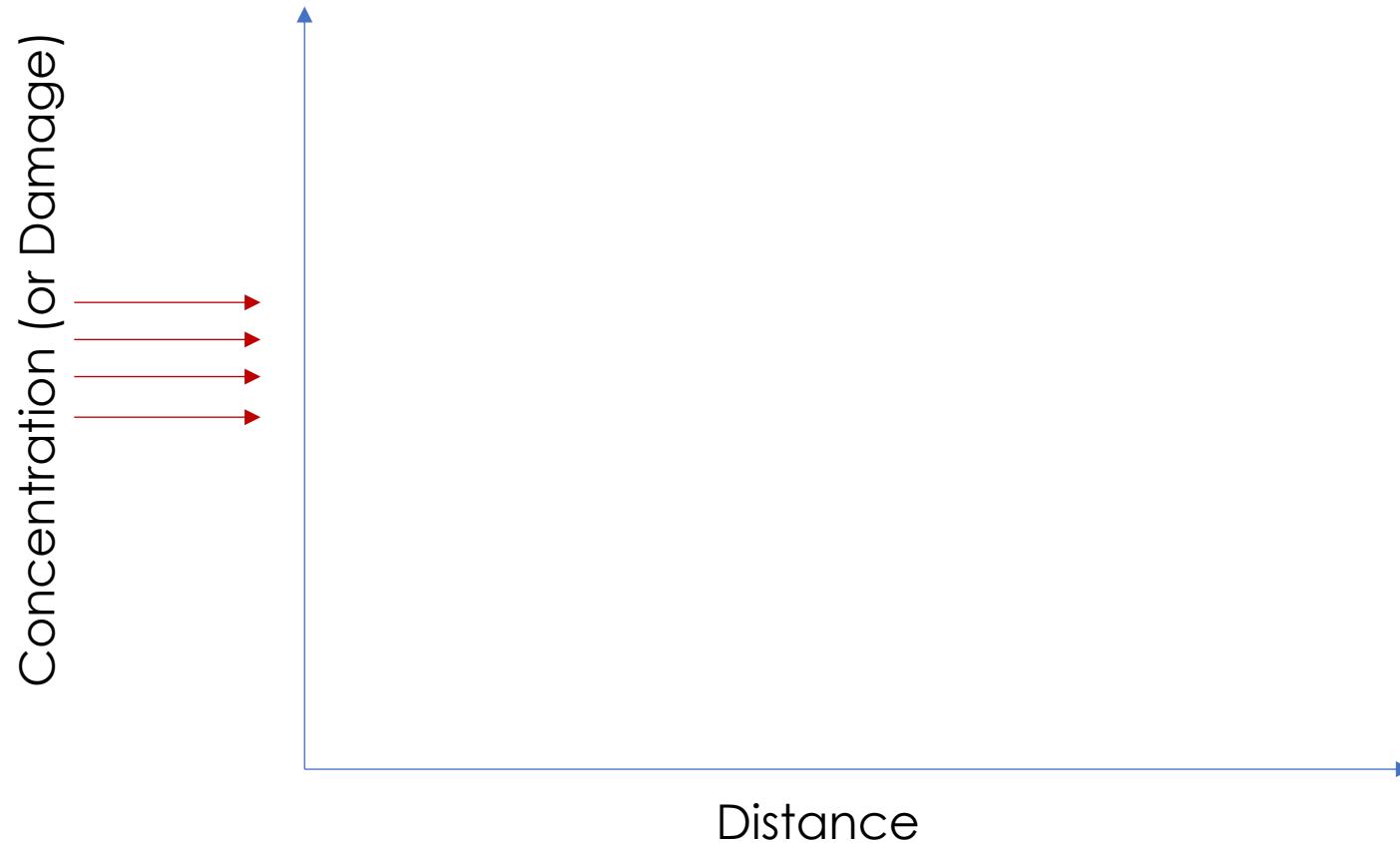
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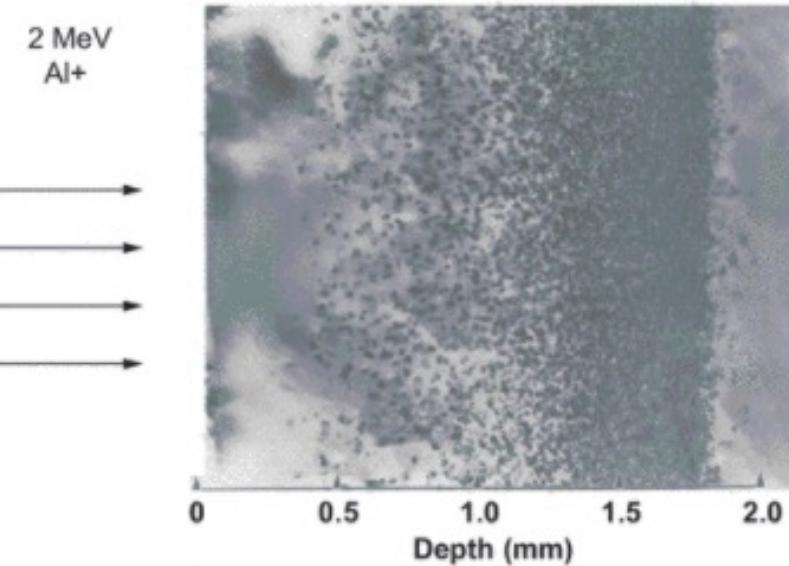
NUCLEAR ENGINEERING &
RADIOLOGICAL SCIENCES
UNIVERSITY OF MICHIGAN

Concentration and Damage

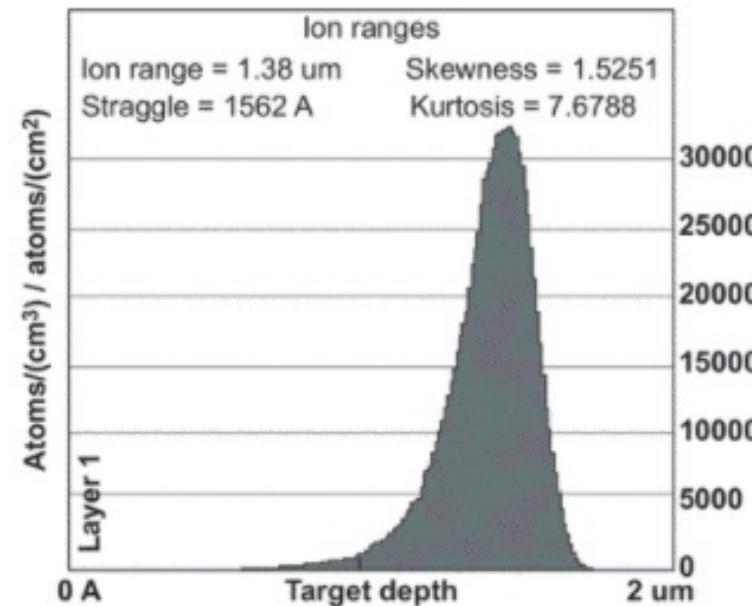


Practical implications of range

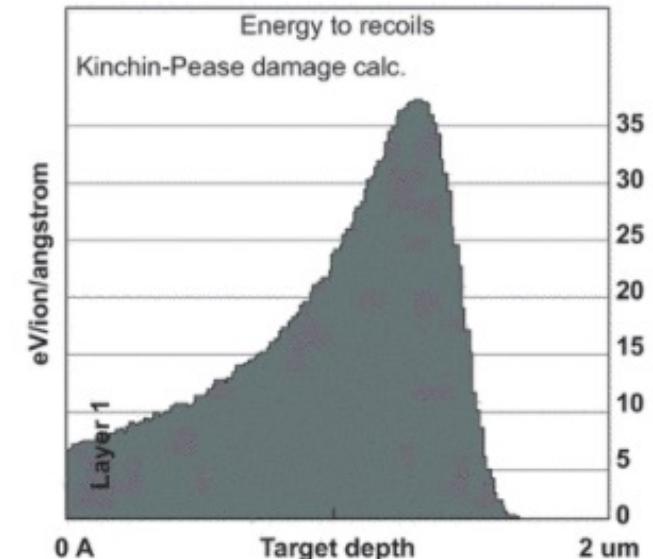
(a)



Microstructure

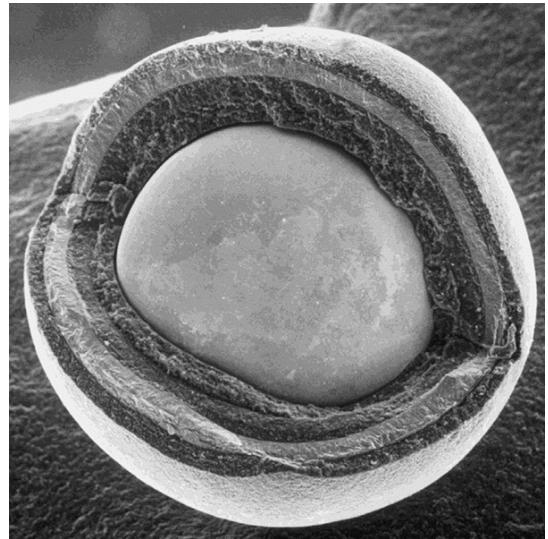


Ion Range

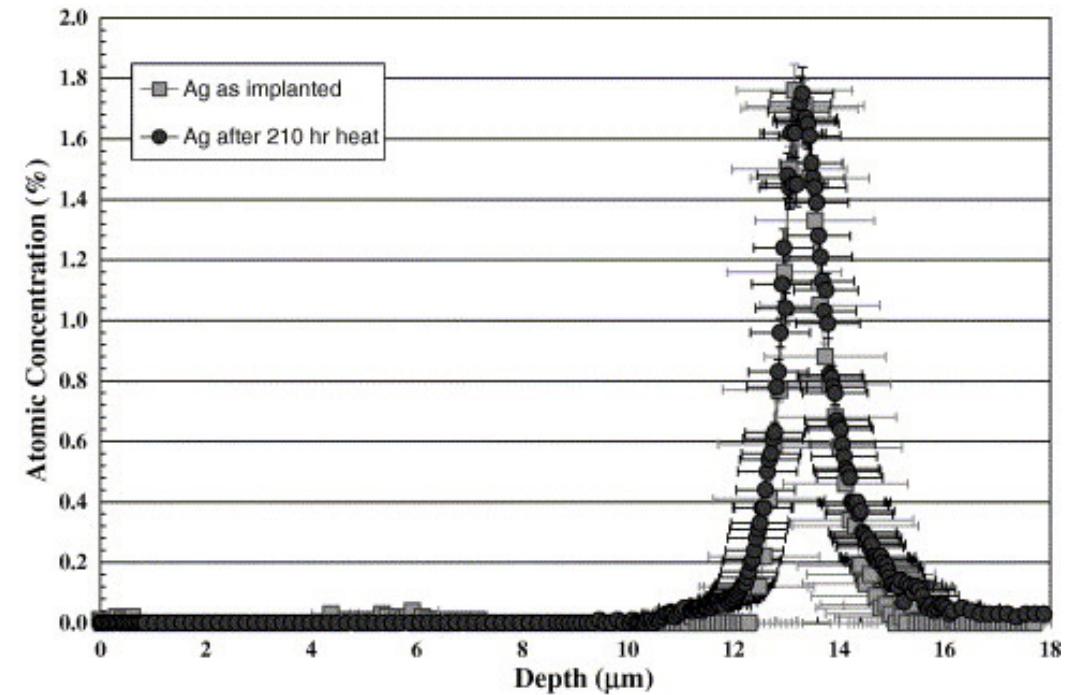
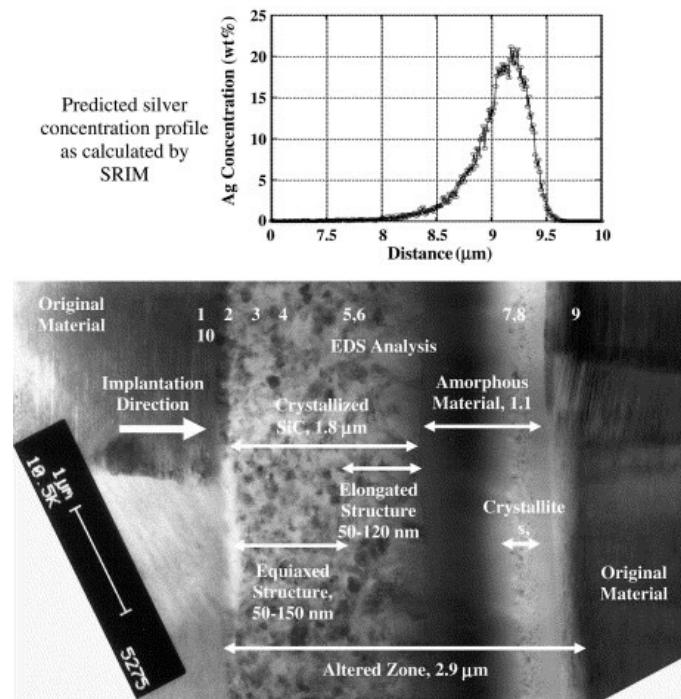


Damage Range

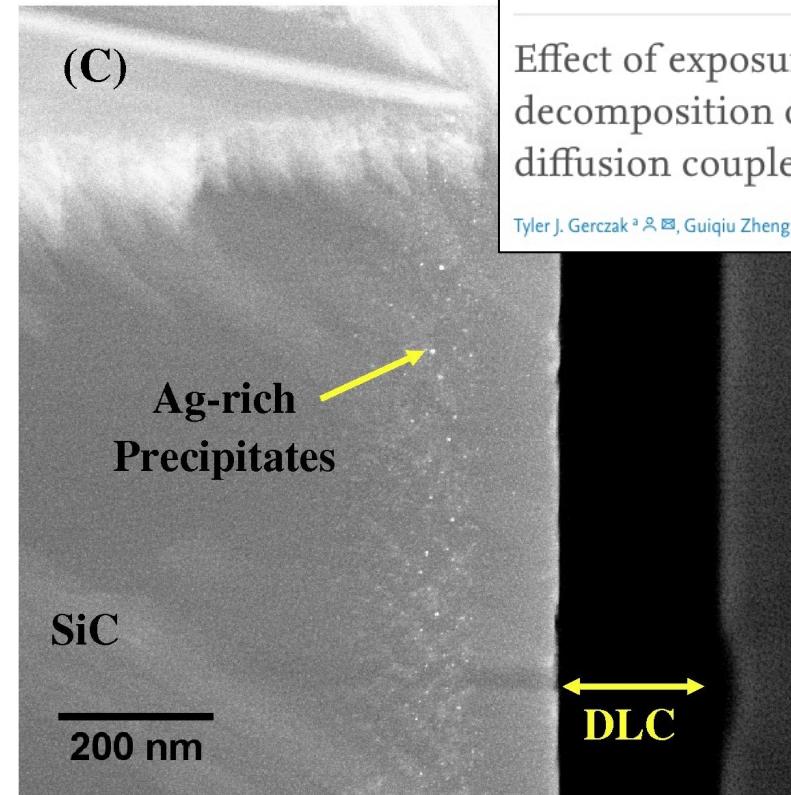
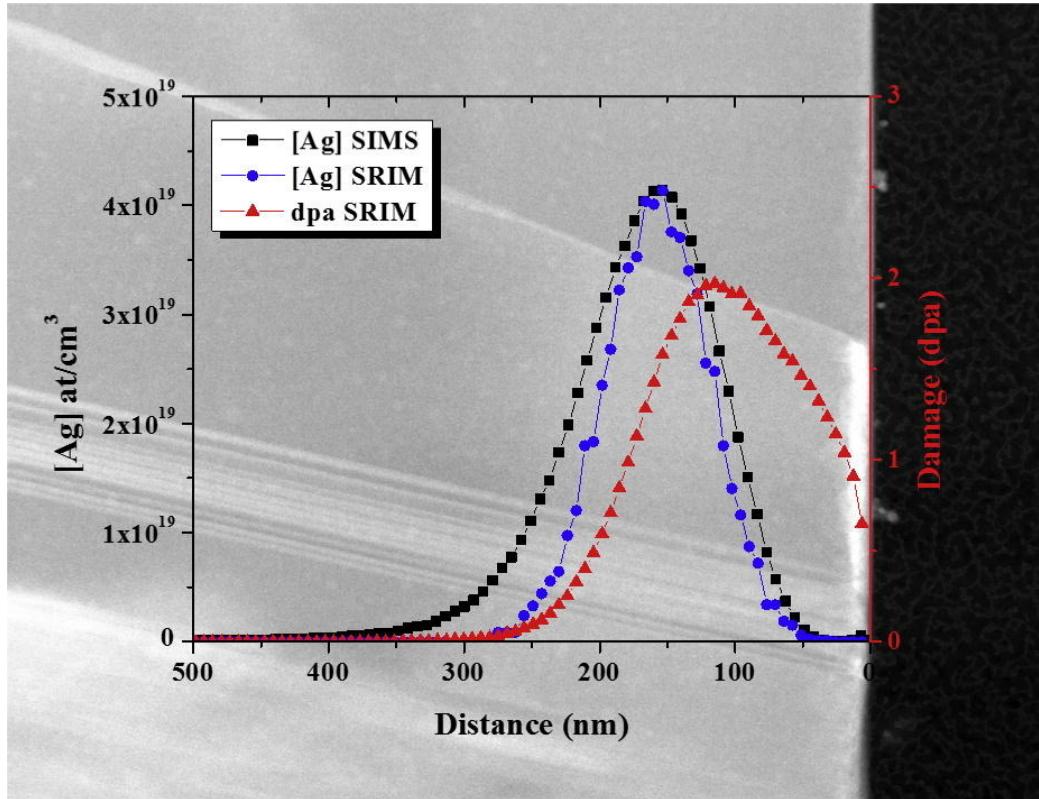
Practical Implications of Range



A TRISO fuel particle



Practical Implications of Range



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

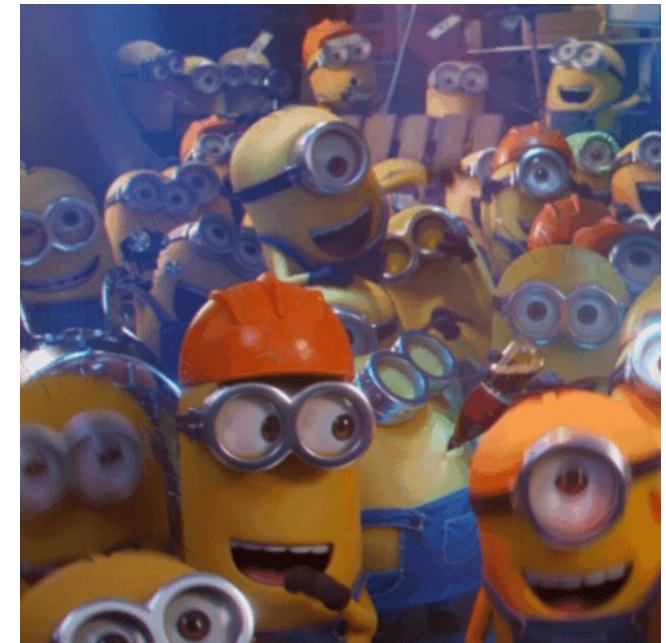
Tyler J. Gerczak ^a✉, Guiqiu Zheng ^a✉, Kevin G. Field ^{b, 1}✉, Todd R. Allen ^c✉

10 citations!

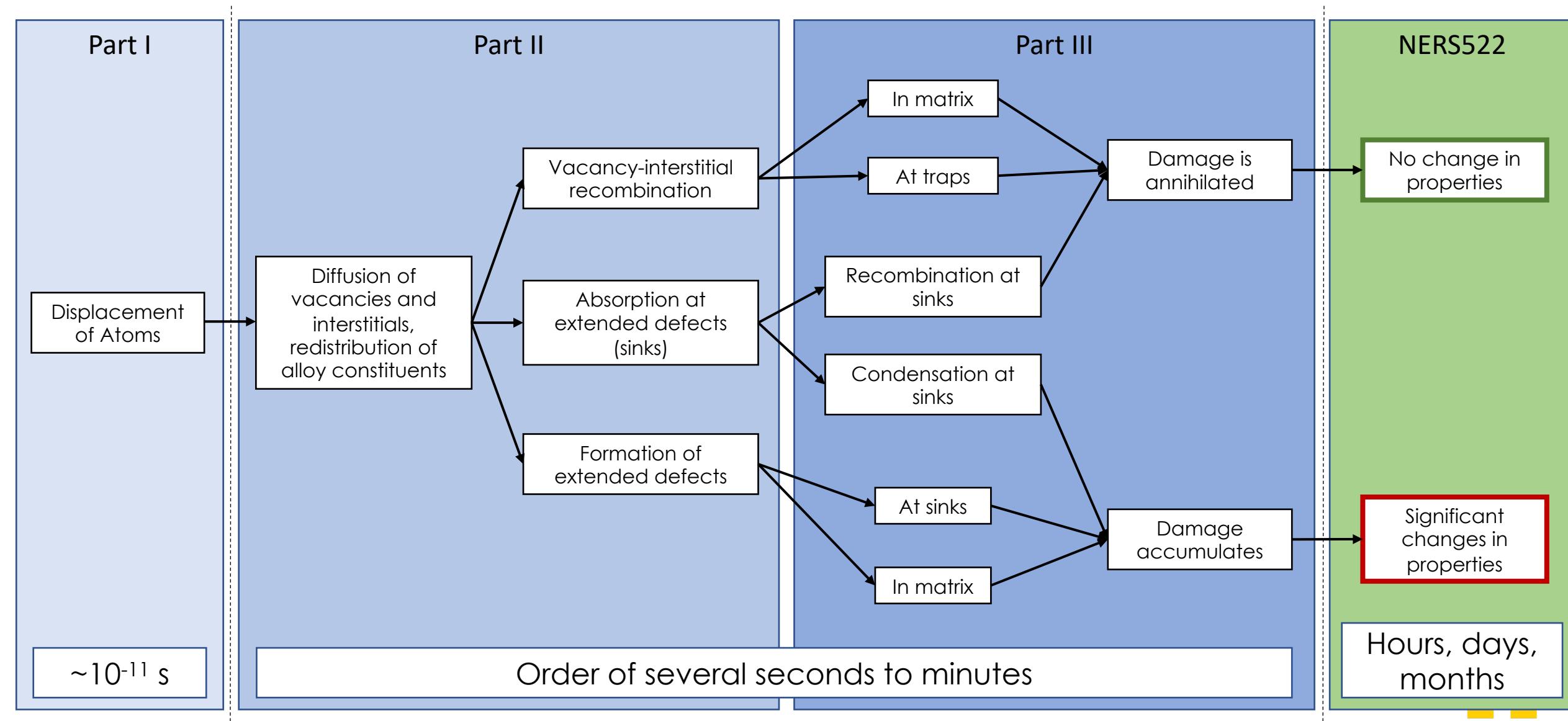


Outline

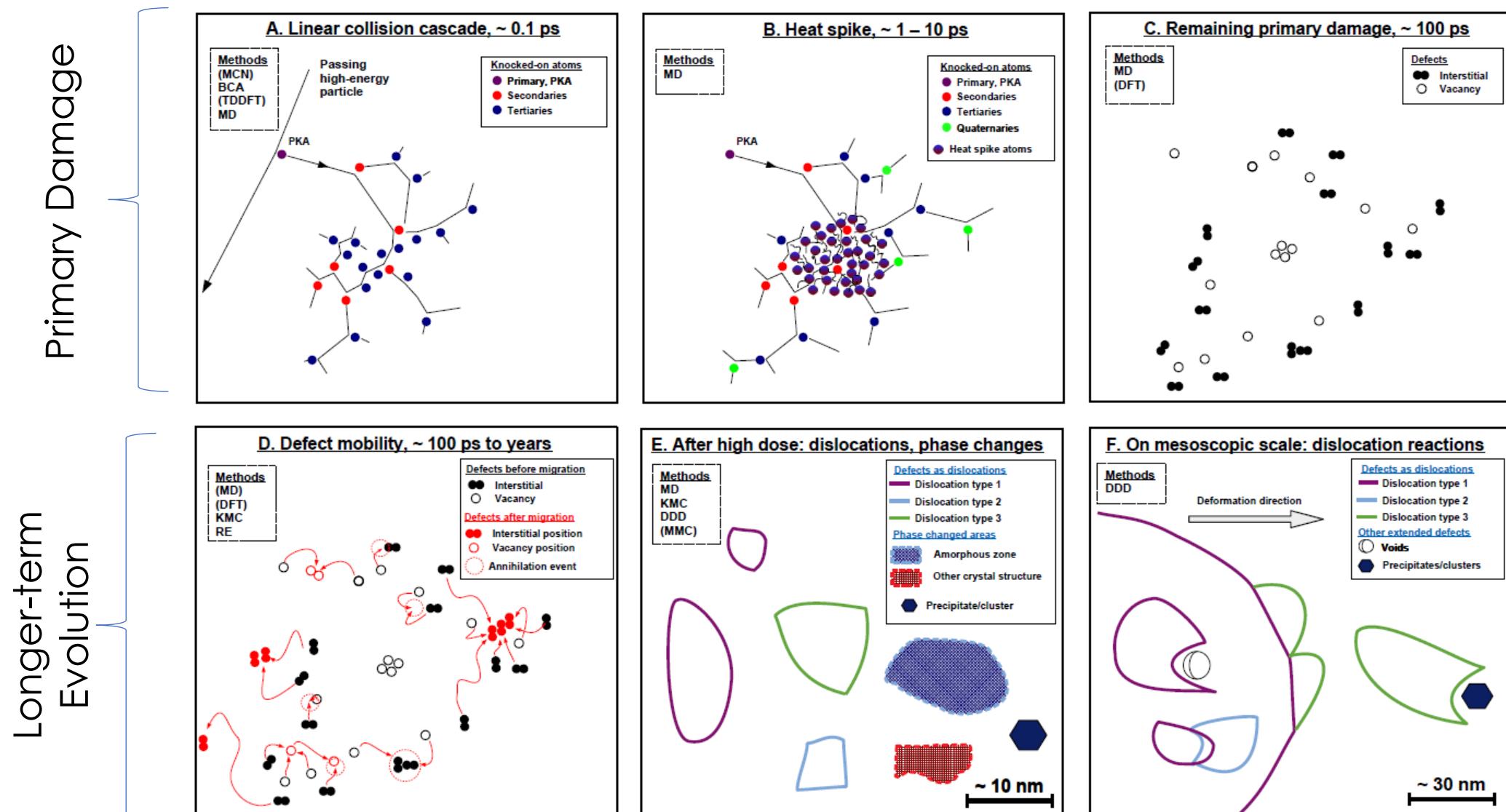
- Multi-collision events or damage **cascades**:
 - When do collisions stop?
 - Rationale for a cascade event
 - Simple picture of the morphology
 - Evolution of a cascade and the resulting effect on materials
- Goal: Understand the damage cascade process and relate that back to determination of dpa



Flow chart for radiation damage



A visual of that flow chart:



Displacement of Atoms in Detail

Part I

Displacement
of Atoms

(Radiation
Damage
Event)

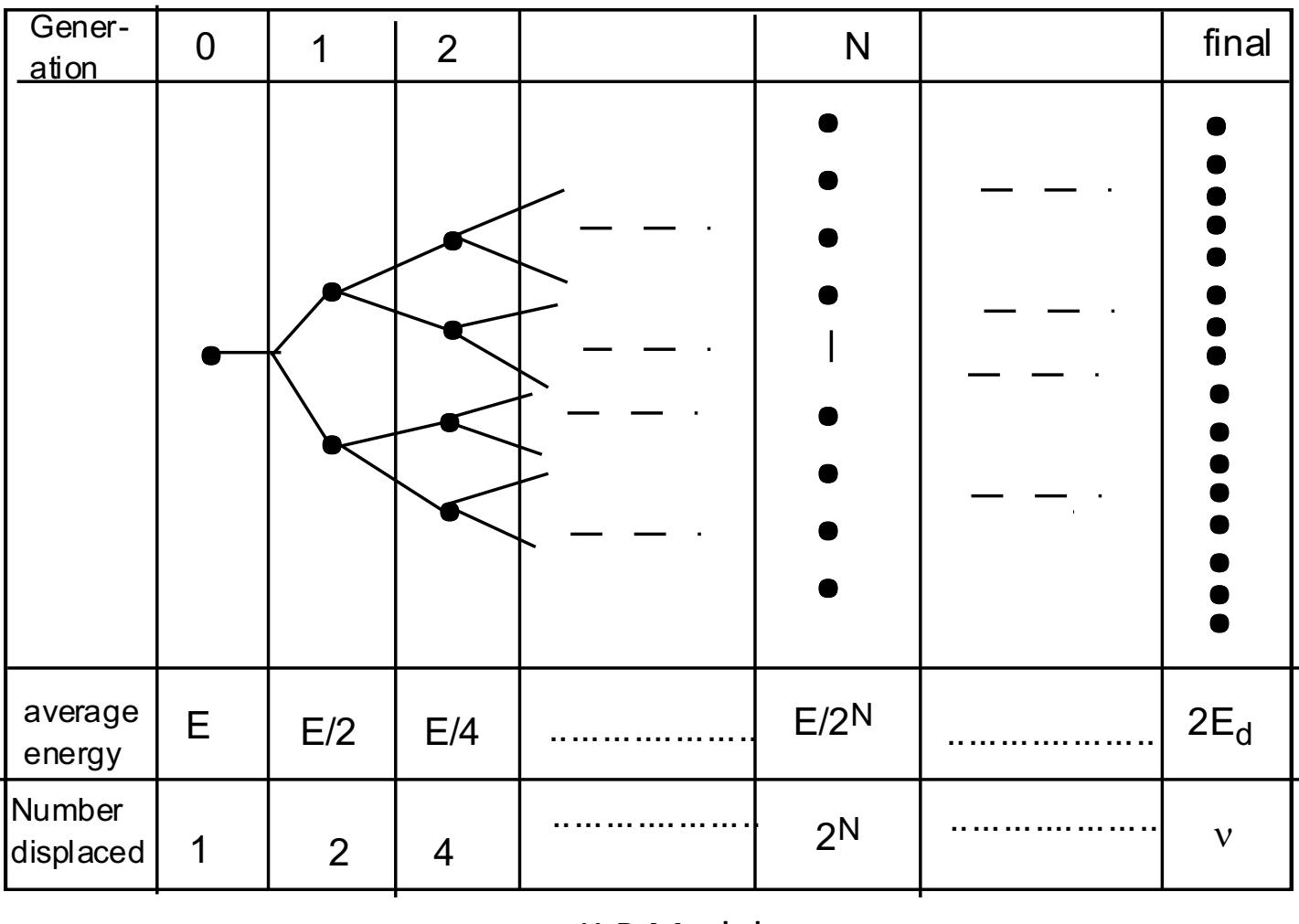
$\sim 10^{-11}$ s

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

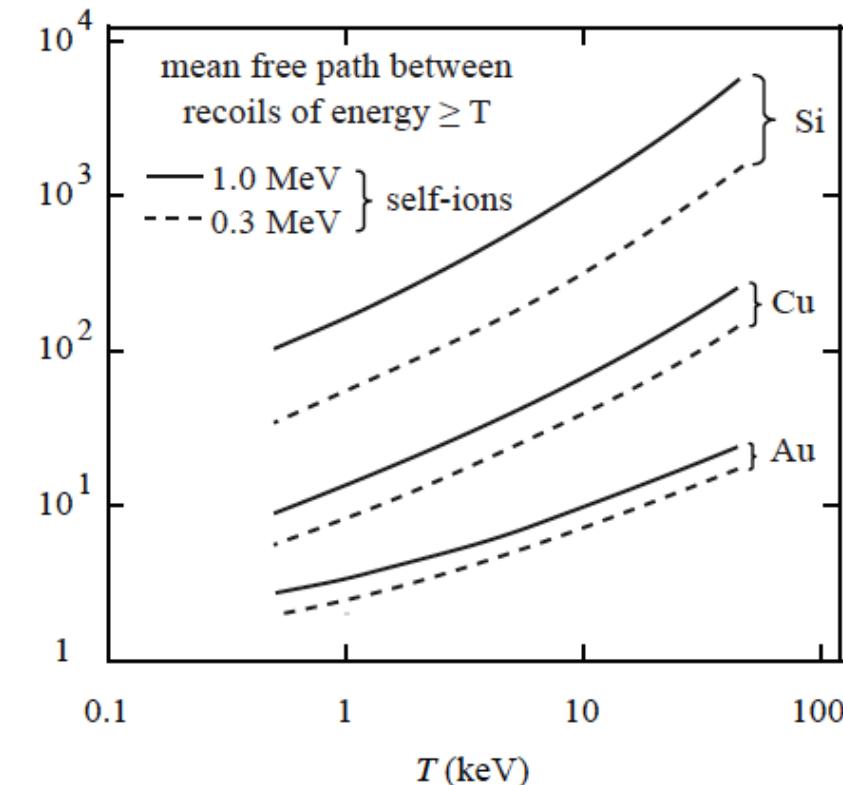
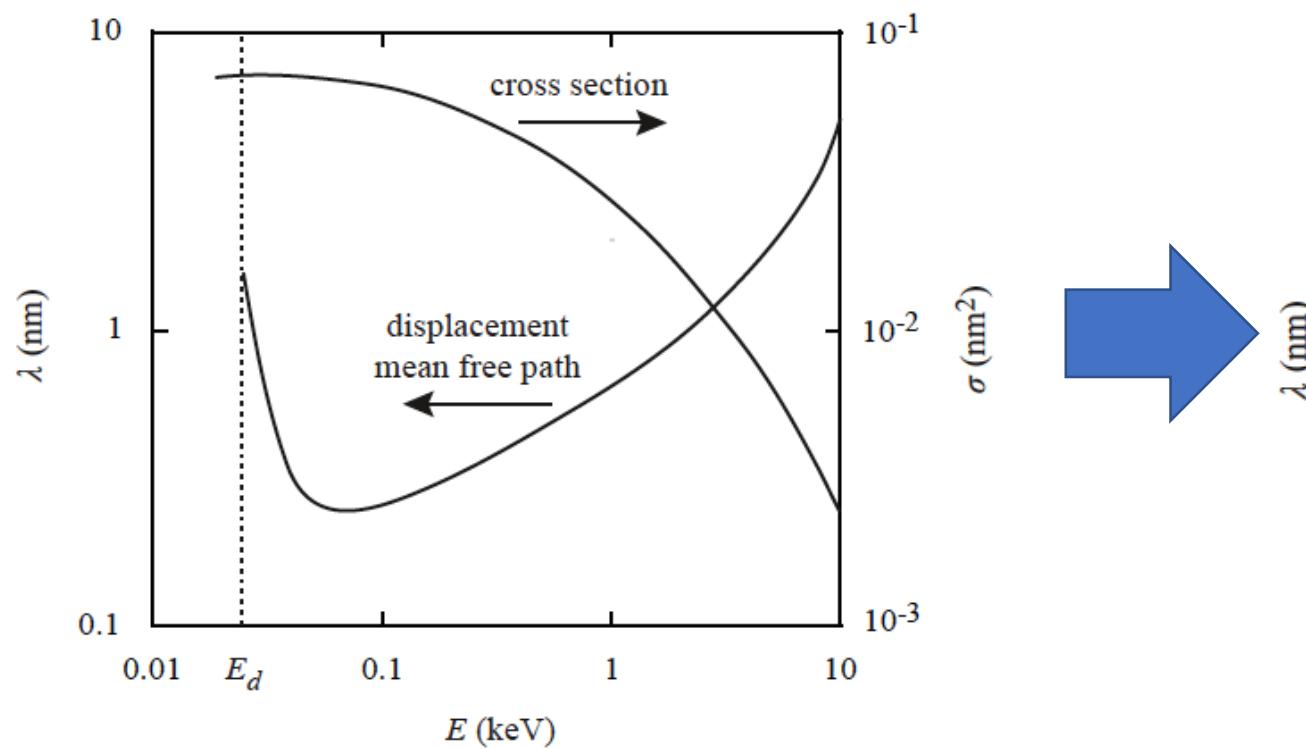
When does a cascade end?

- Remember:
 - Cascade ceases when knock-on energy is:



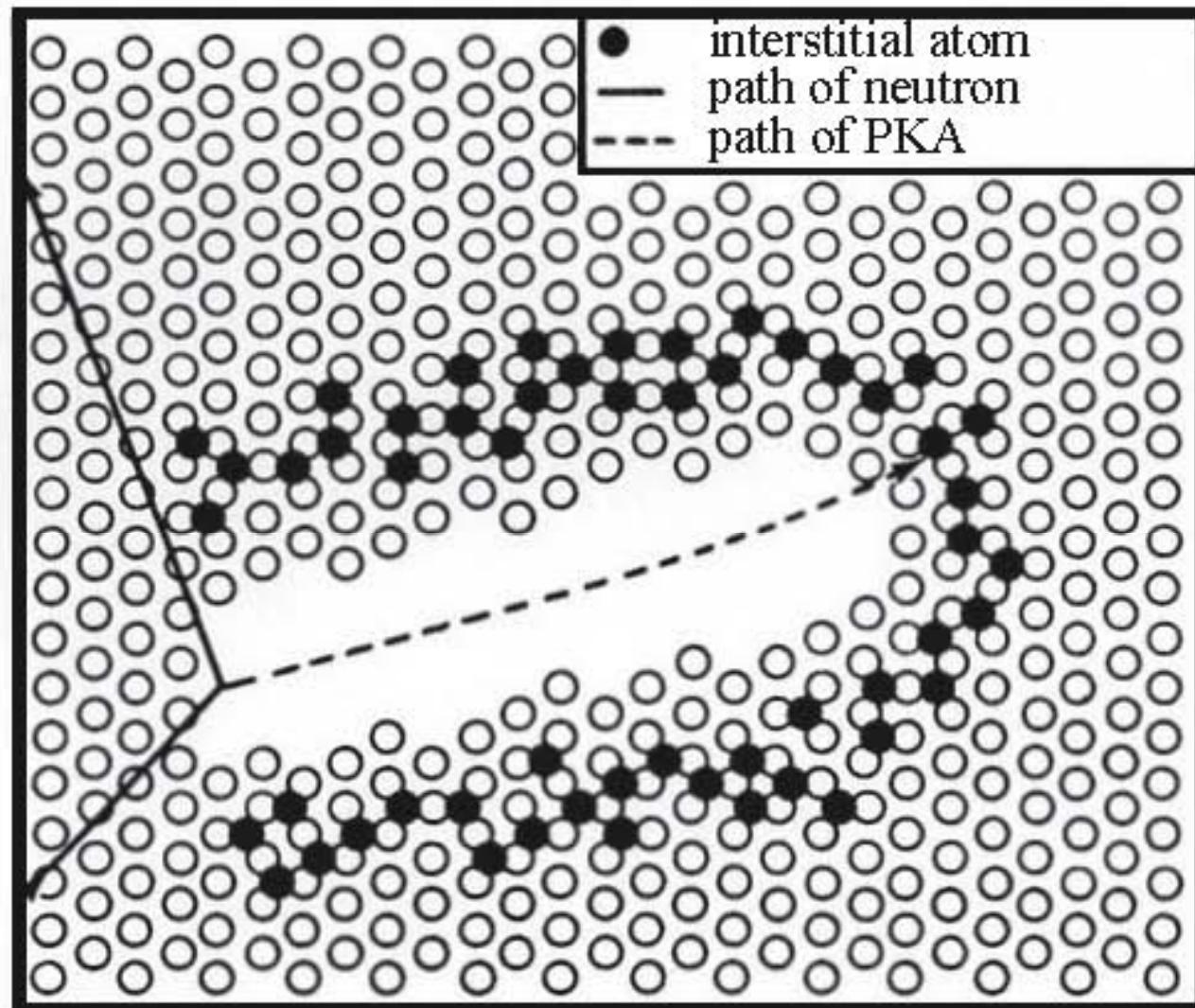
Mean free path between recoils

- 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

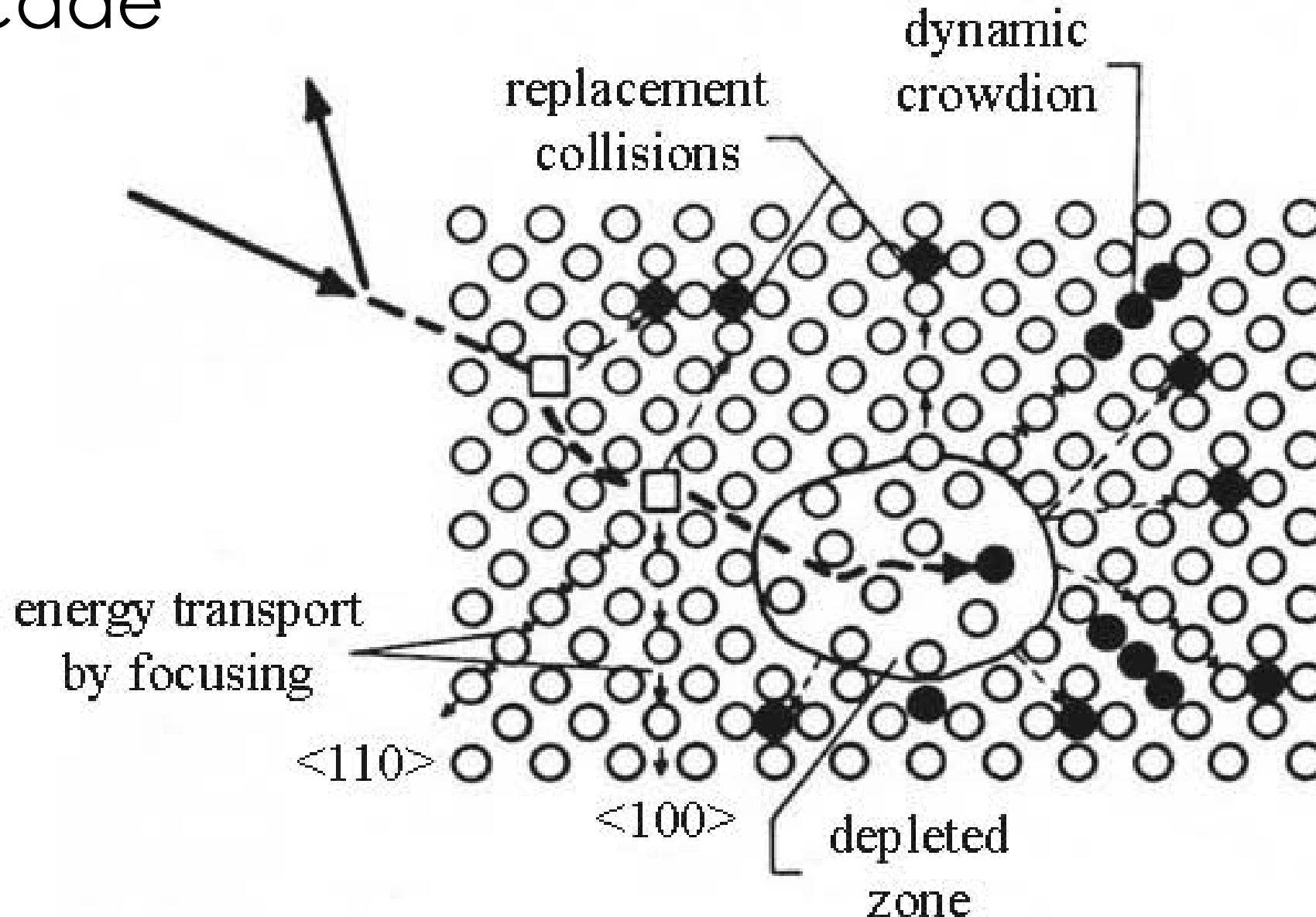


Original conception of the damage cascade

Use the term “damage cascade” to signify the continued damage effects from PKA, SKA, etc...

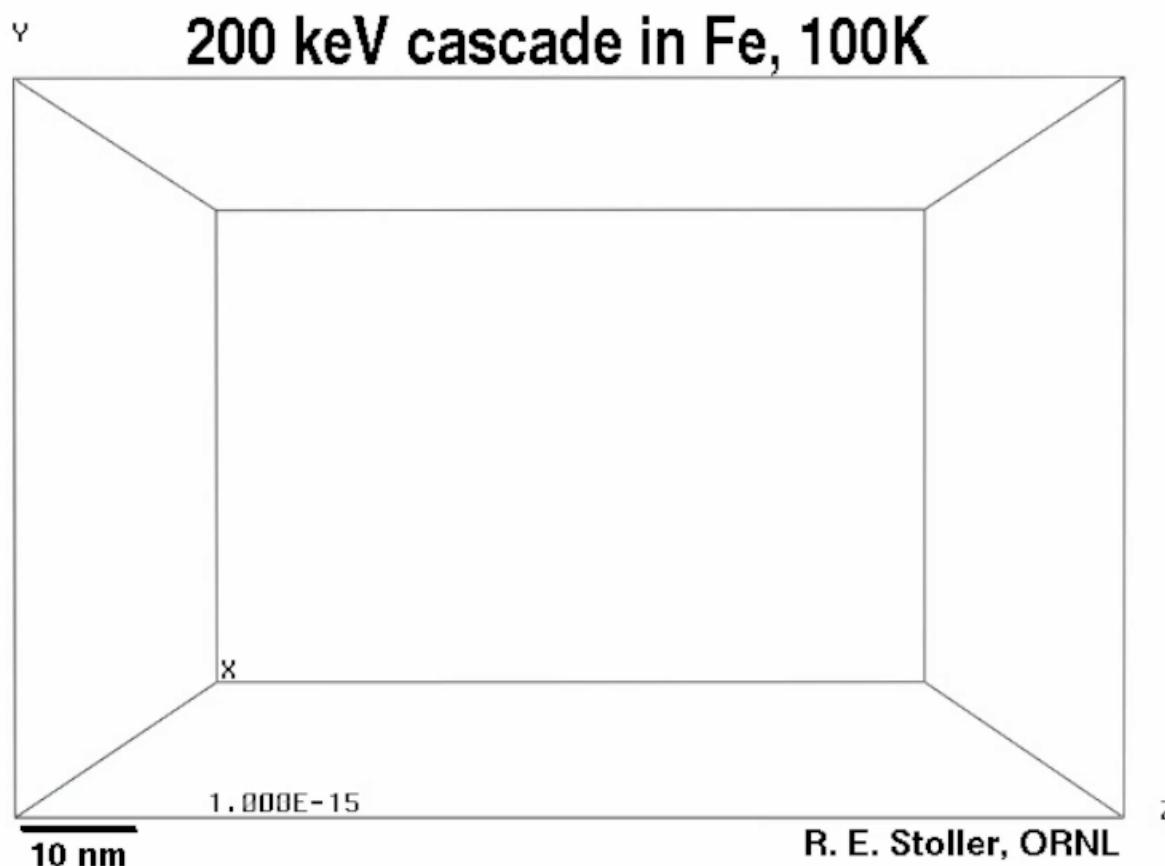


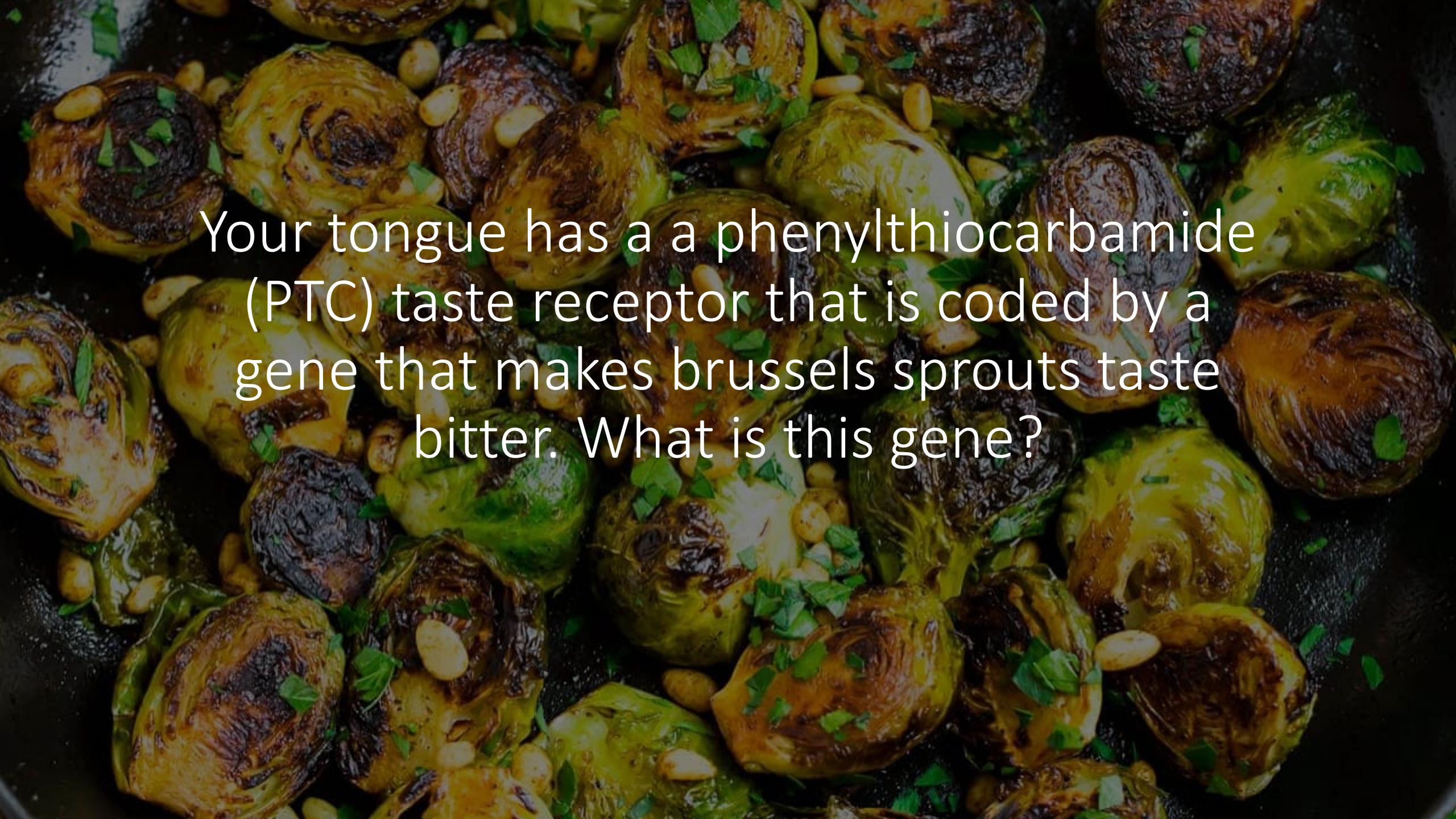
Another revised conception of the damage cascade



A more realistic visual:

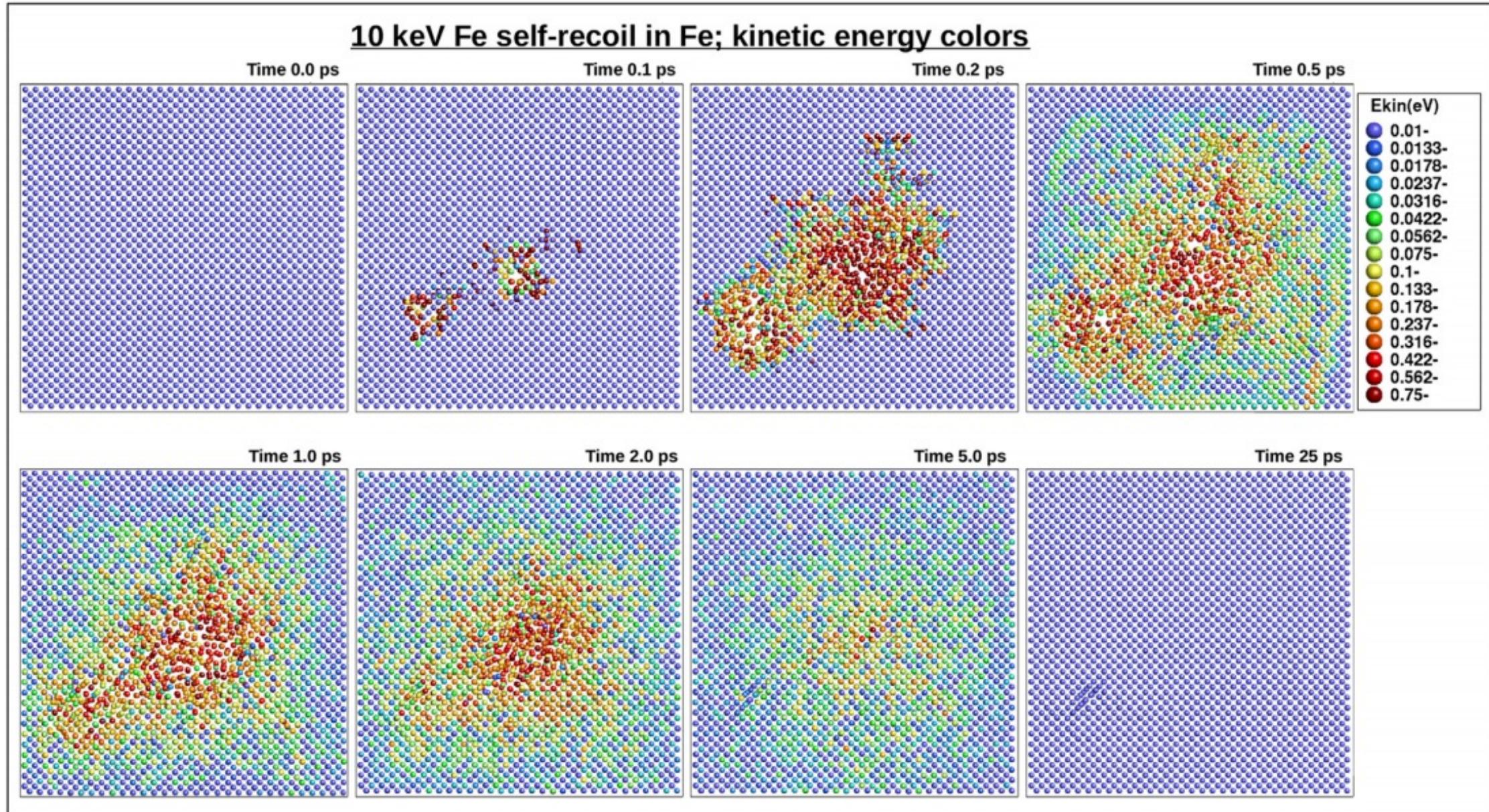
3.1 Molecular Dynamics (MD) simulation of the development of a cascade from a 20 keV recoil in iron at 100K. Note the striking difference in defect density between the peak of the ballistic regime (~ 1 ps) and that at the end of the quench (~ 5 ps). (courtesy, R. Stoller, Oak Ridge National Laboratory)



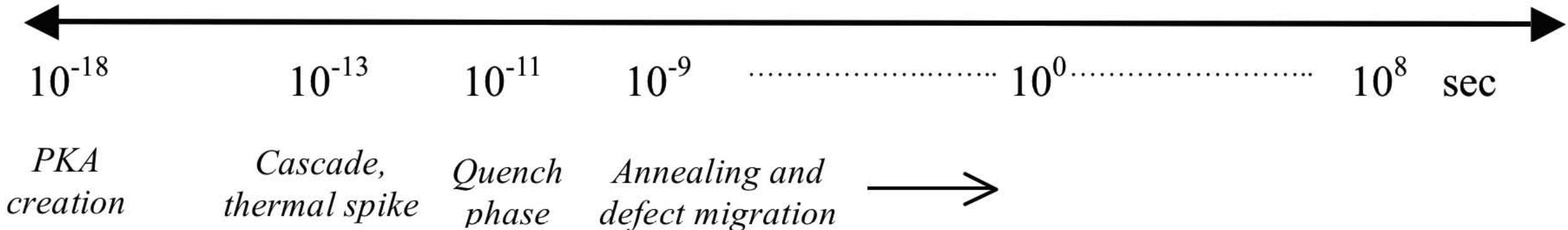
A close-up photograph of roasted Brussels sprouts. The sprouts are golden brown and caramelized, with some darker, charred edges. They are garnished with finely chopped green herbs, likely parsley or chives, and small, light-colored pine nuts. The lighting highlights the texture of the roasted vegetables against a dark, possibly black, background.

Your tongue has a phenylthiocarbamide (PTC) taste receptor that is coded by a gene that makes brussels sprouts taste bitter. What is this gene?

Visual snapshot of a cascade and stages



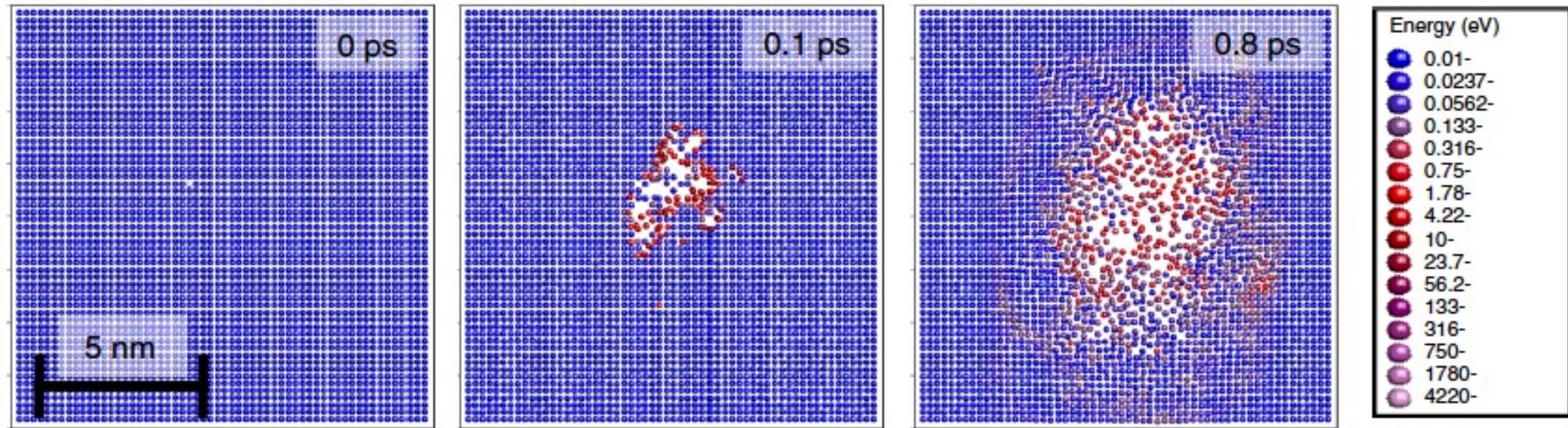
Cascades have four distinct stages:



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



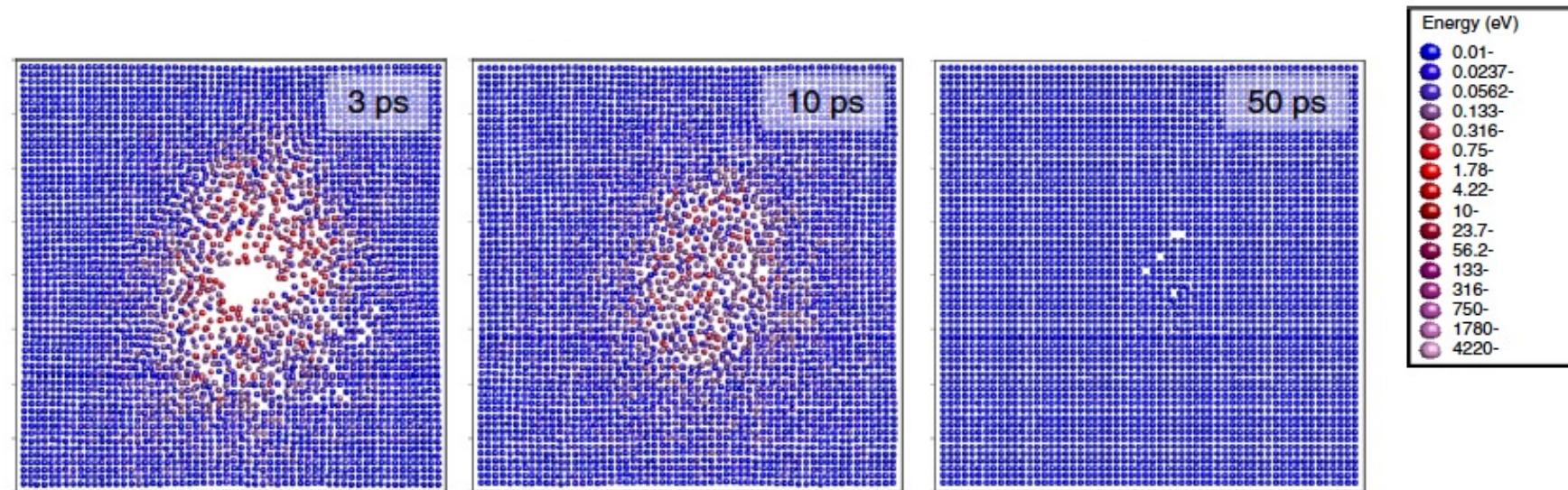
Collisional -> Thermal Spike



- 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

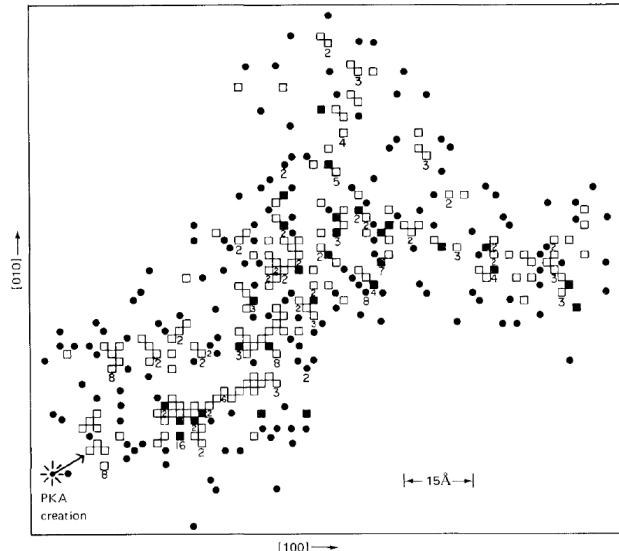


Fig. 17.27 Displacement spike due to a 20-keV PKA in iron projected onto the (001) plane (0°K). [After J. R. Beeler, Jr., *Phys. Rev.*, **150**: 470 (1966).]

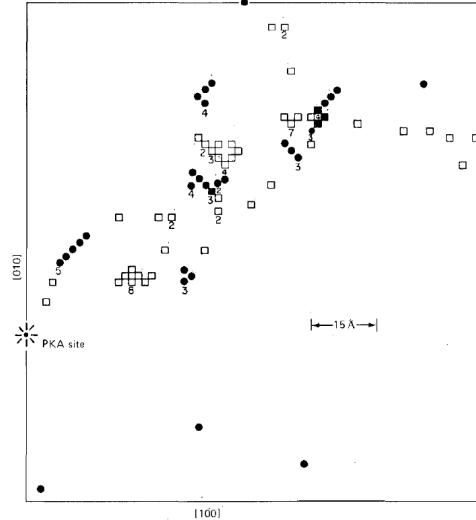


Fig. 17.28 Displacement spike [projected onto the (001) plane] due to a 20-keV PKA in iron after annealing at 800°K (6000 interstitial jumps and 60 vacancy jumps). The preannealed spike is shown in Fig. 17.27. Numbers on the diagram denote cluster sizes. Twelve interstitials have migrated outside the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

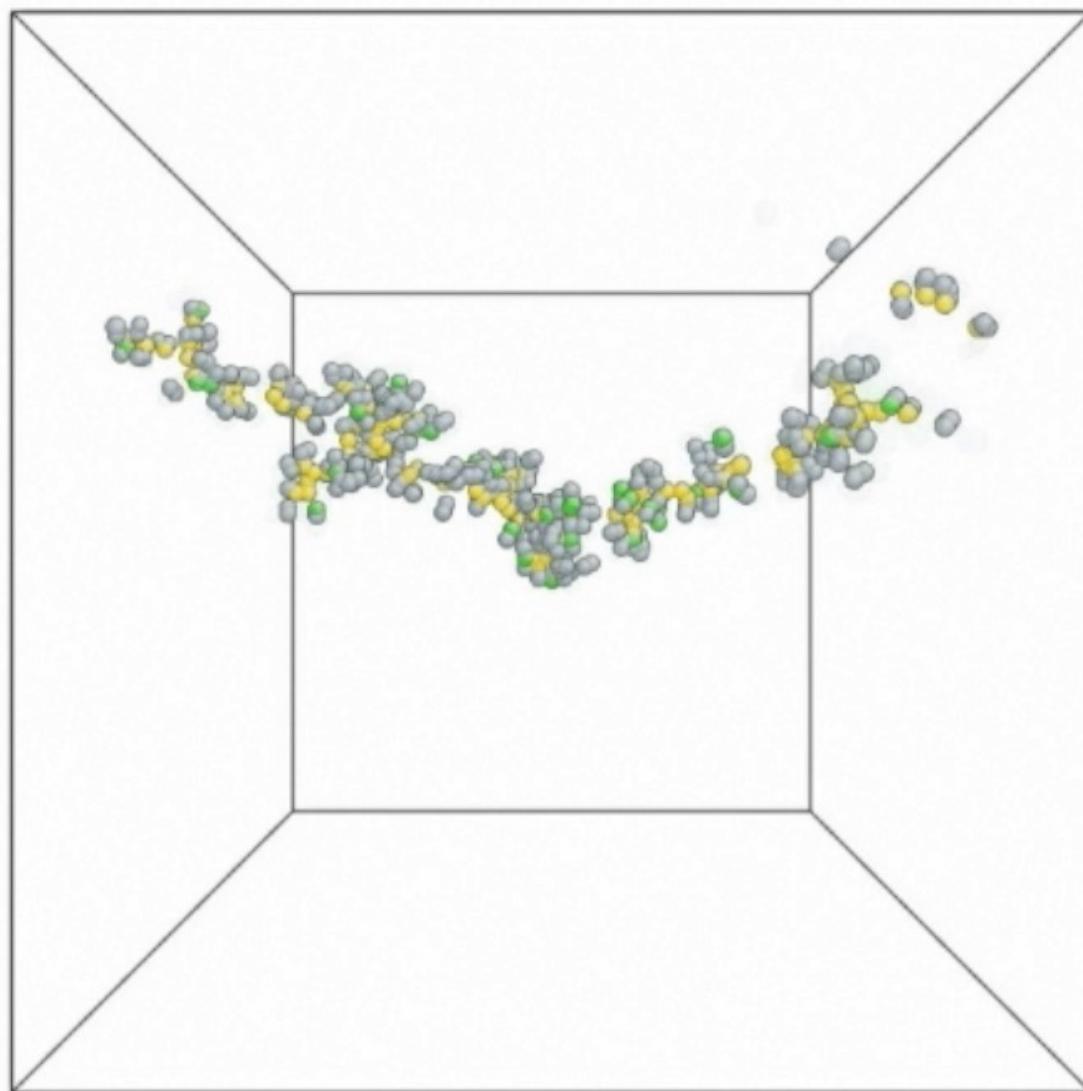
- Annealing can be simply evaluated by looking at the jump rate, where interstitials are enabled to jump to different lattice sites more frequently. The following possibilities can happen:
 - Point defect jumps into a recombination volume around a point defect of opposite sign -> the two are annihilated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



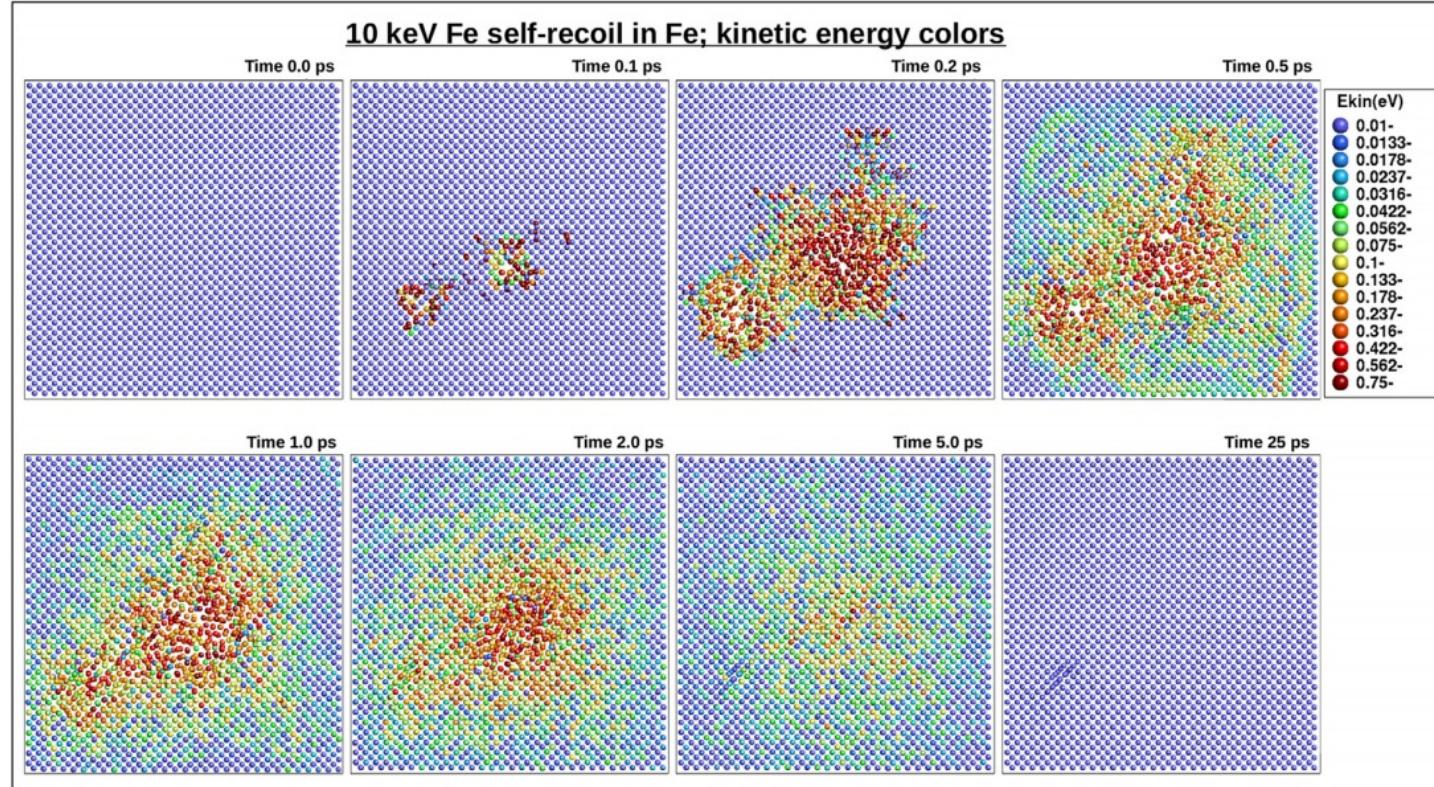
A more realistic visual:

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)



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

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 ion-range interstitial mobility from nearby collision cascade

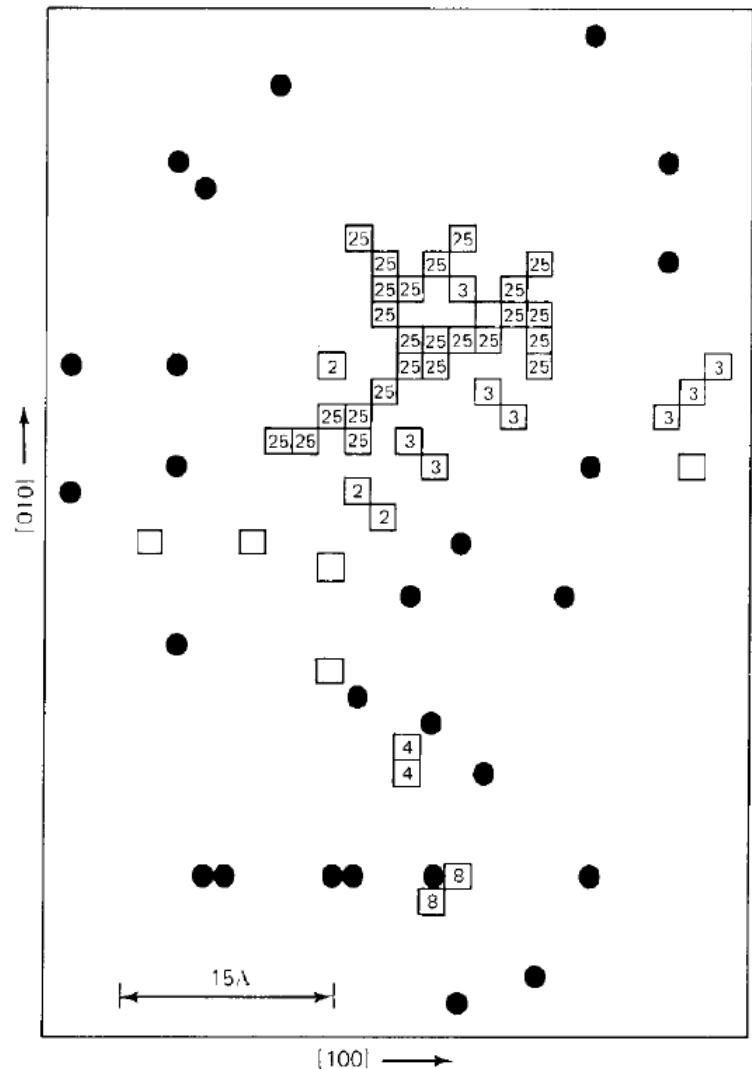


Fig. 17.30 A 25-vacancy cluster formed by the overlap of three successive 5-keV displacement spikes in copper (0°K). (After Ref. 30.)



Different radiation produces different cascades

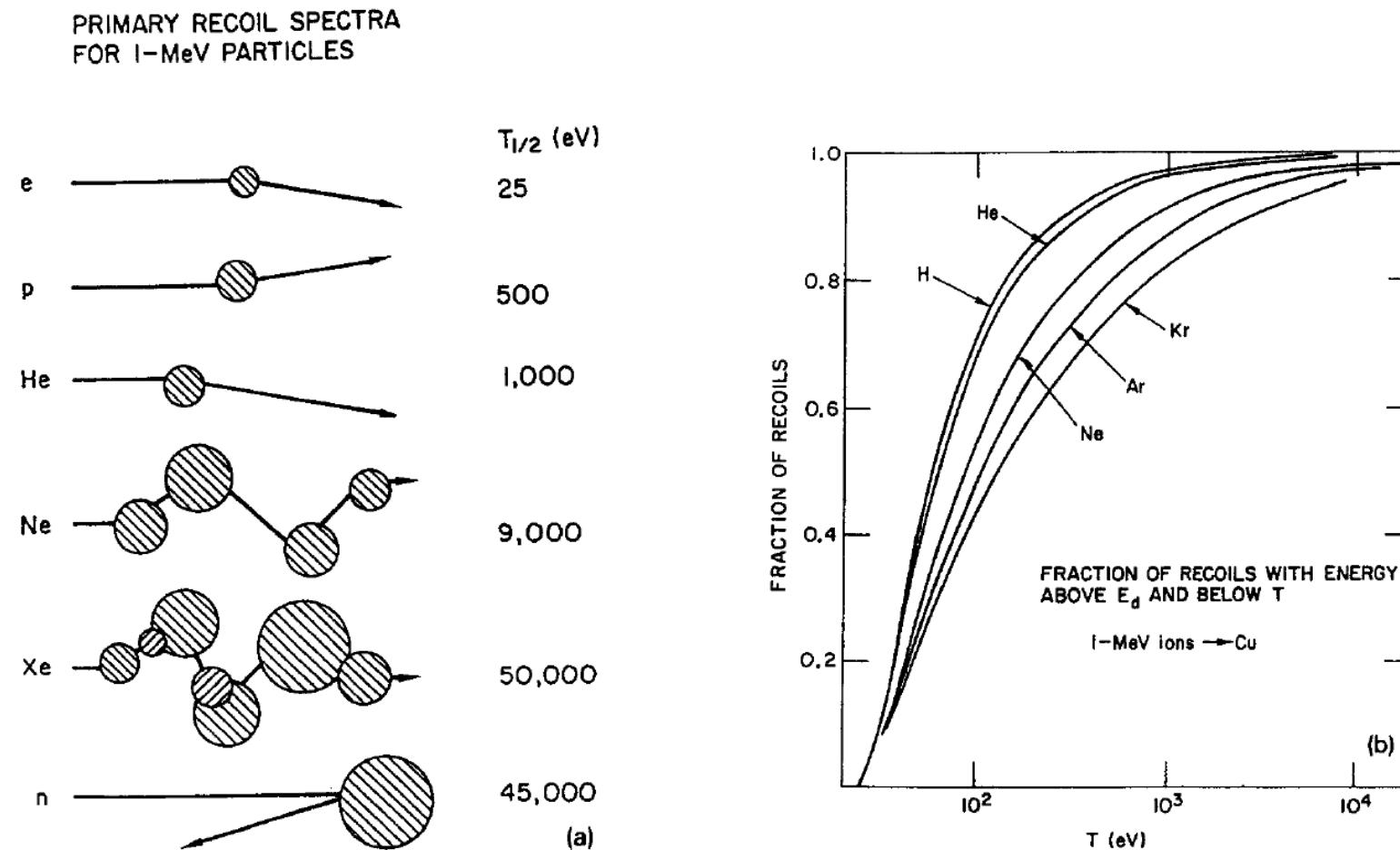


Fig. 2. (a) Qualitative representation of the primary recoil spectra for 1 MeV particles in Cu. Circles indicate where energetic recoils occur and their size indicates the amount of energy transferred to the recoil atom. $T_{1/2}$ refers to a “typical” recoil energy which is defined below. (b) Integral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

Different radiation produces different cascades

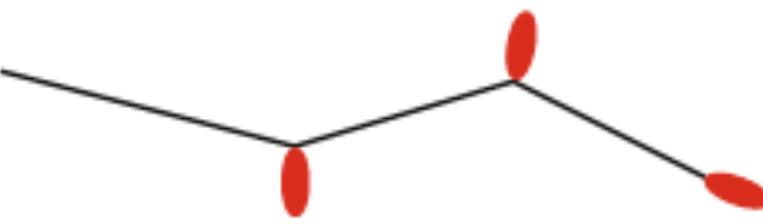
Mass & Charge:

1 MeV electrons
 $\bar{T} = 60 \text{ eV}$
 $\xi = 50 - 100\%$

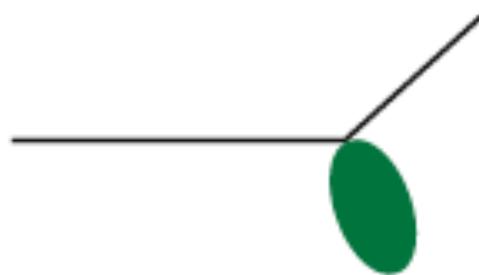


Increasing mass, same charge

1 MeV protons
 $\bar{T} = 200 \text{ eV}$
 $\xi = 25\%$

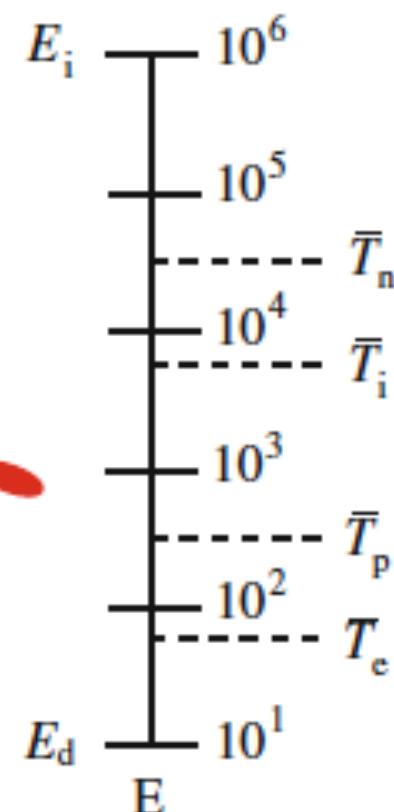


1 MeV heavy ions
 $\bar{T} = 5 \text{ keV}$
 $\xi = 4\%$



Moderate mass, no charge

1 MeV neutrons
 $\bar{T} = 35 \text{ keV}$
 $\xi = 2\%$



Stopping mechanism:



Displacement Efficiency

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

$$\xi = \delta_i + \eta_i + \eta_{i,v} = \delta_v + \eta_v + \eta_{v,i}$$

$\eta_{i,v}$ = isolated point defect fraction

$\delta_{i,v}$ = clustered fraction including mobile defect clusters

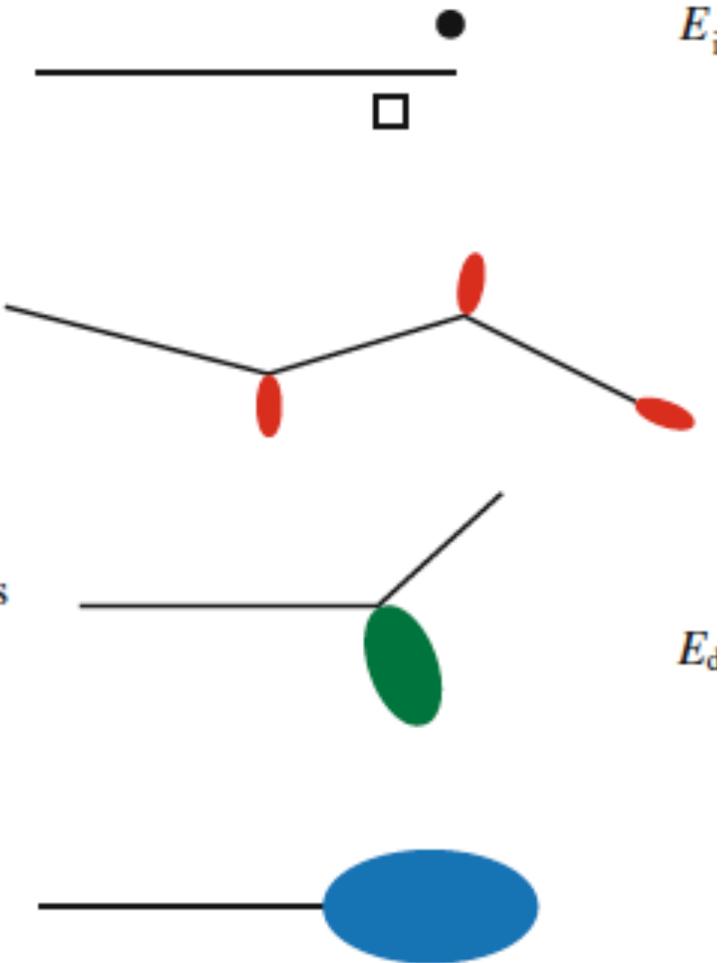
ξ = fraction initially in isolated or clustered form after the cascade quench that is annihilated during subsequent short term ($> 10^{-11}$ s) intracascade thermal diffusion

1 MeV electrons
 $\bar{T} = 60$ eV
 $\xi = 50 - 100\%$

1 MeV protons
 $\bar{T} = 200$ eV
 $\xi = 25\%$

1 MeV heavy ions
 $\bar{T} = 5$ keV
 $\xi = 4\%$

1 MeV neutrons
 $\bar{T} = 35$ keV
 $\xi = 2\%$



Displacement Efficiency

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

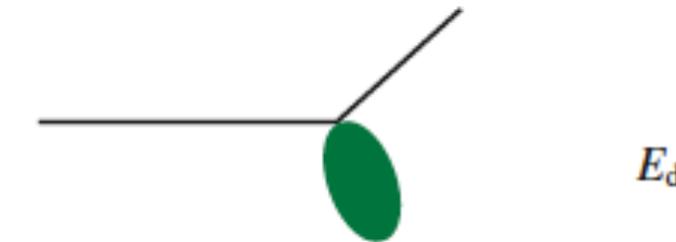
1 MeV electrons
 $\bar{T} = 60 \text{ eV}$
 $\xi = 50\text{--}100\%$



1 MeV protons
 $\bar{T} = 200 \text{ eV}$
 $\xi = 25\%$



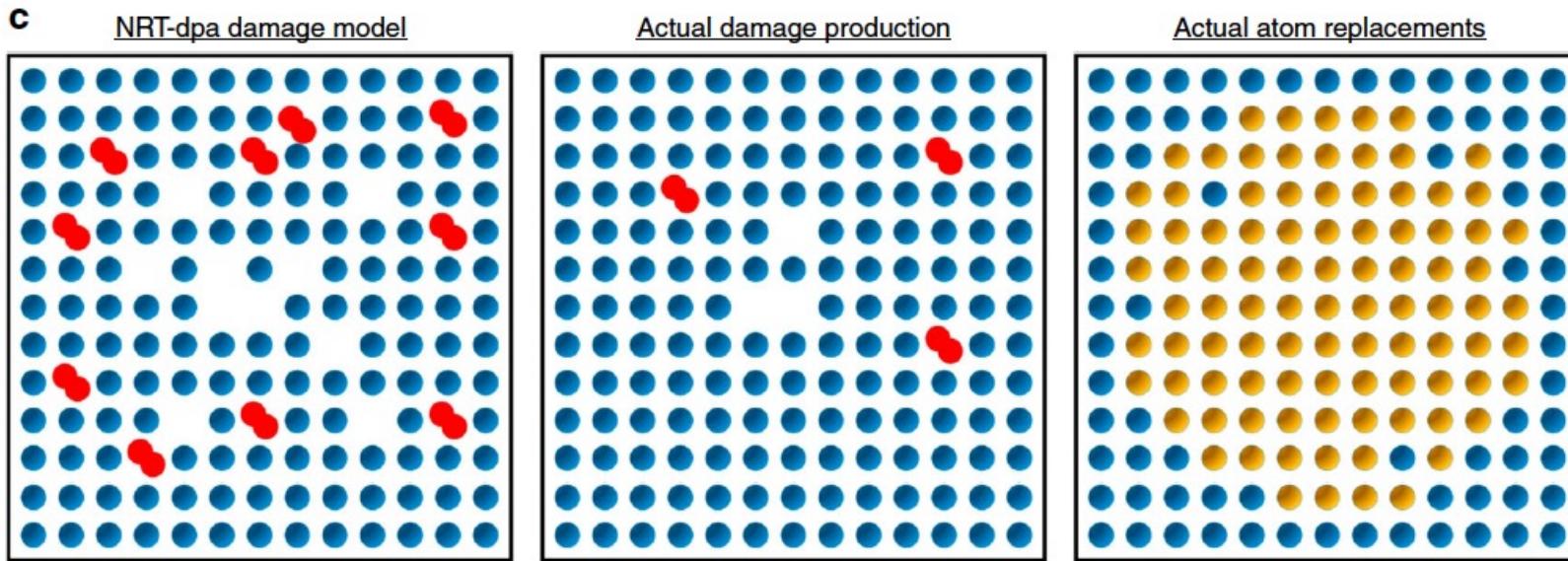
1 MeV heavy ions
 $\bar{T} = 5 \text{ keV}$
 $\xi = 4\%$



1 MeV neutrons
 $\bar{T} = 35 \text{ keV}$
 $\xi = 2\%$



Modification to NRT model based on cascade physics



Arc-dpa: Athermal recombination corrected dpa

- Accounts for enhanced recombination in metals in a cascade

Rpa: Replacements per atom

- Provides a measure of the volume of irradiated material directly affected by the cascade
 - Implications on phase stability and mixing



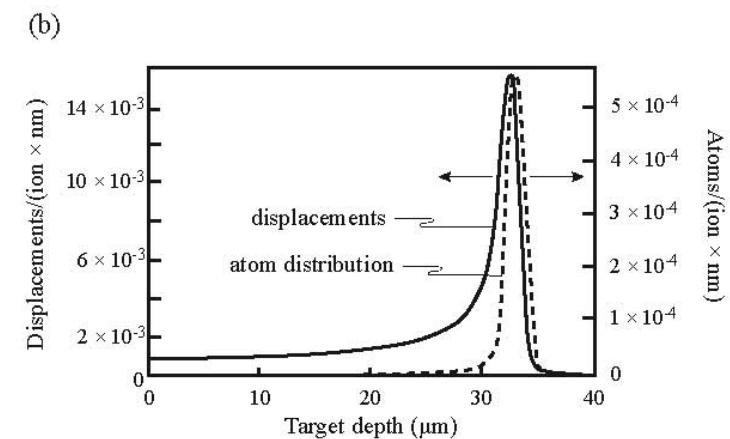
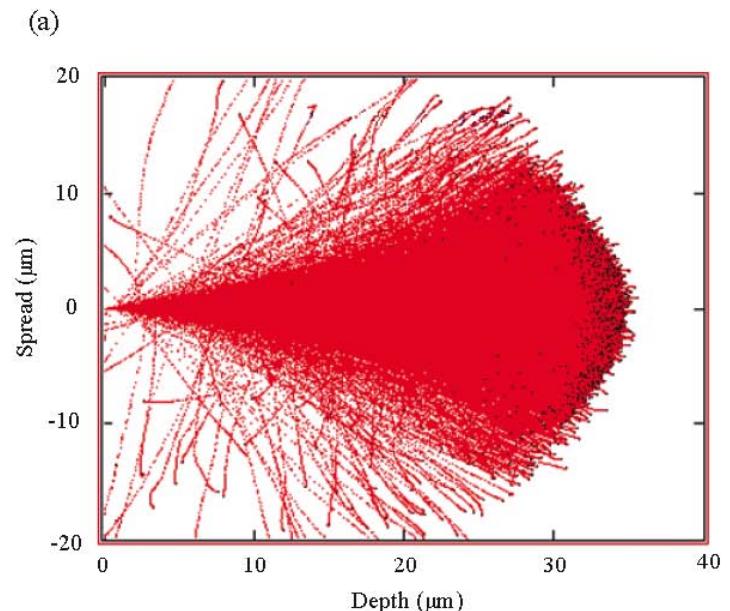
Simulation methods – Monte Carlo

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!



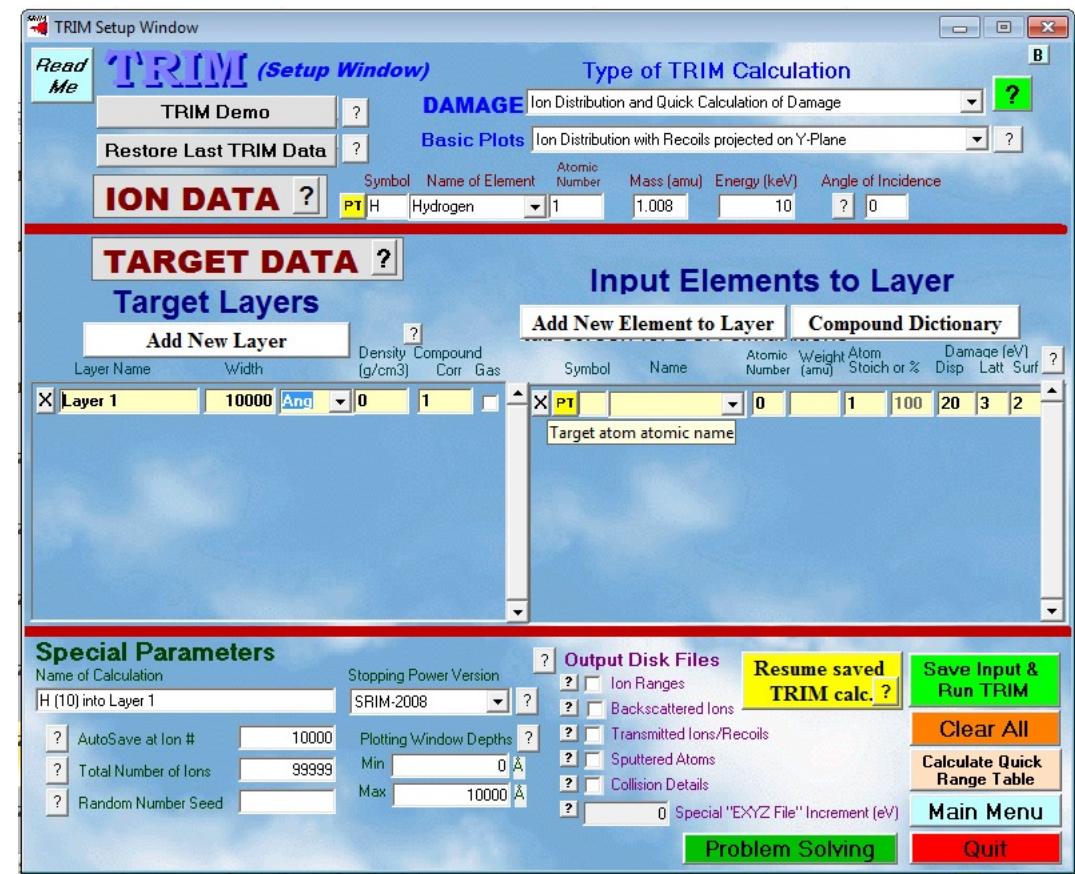
The SRIM software

The SRIM software is freely available at the SRIM web pages

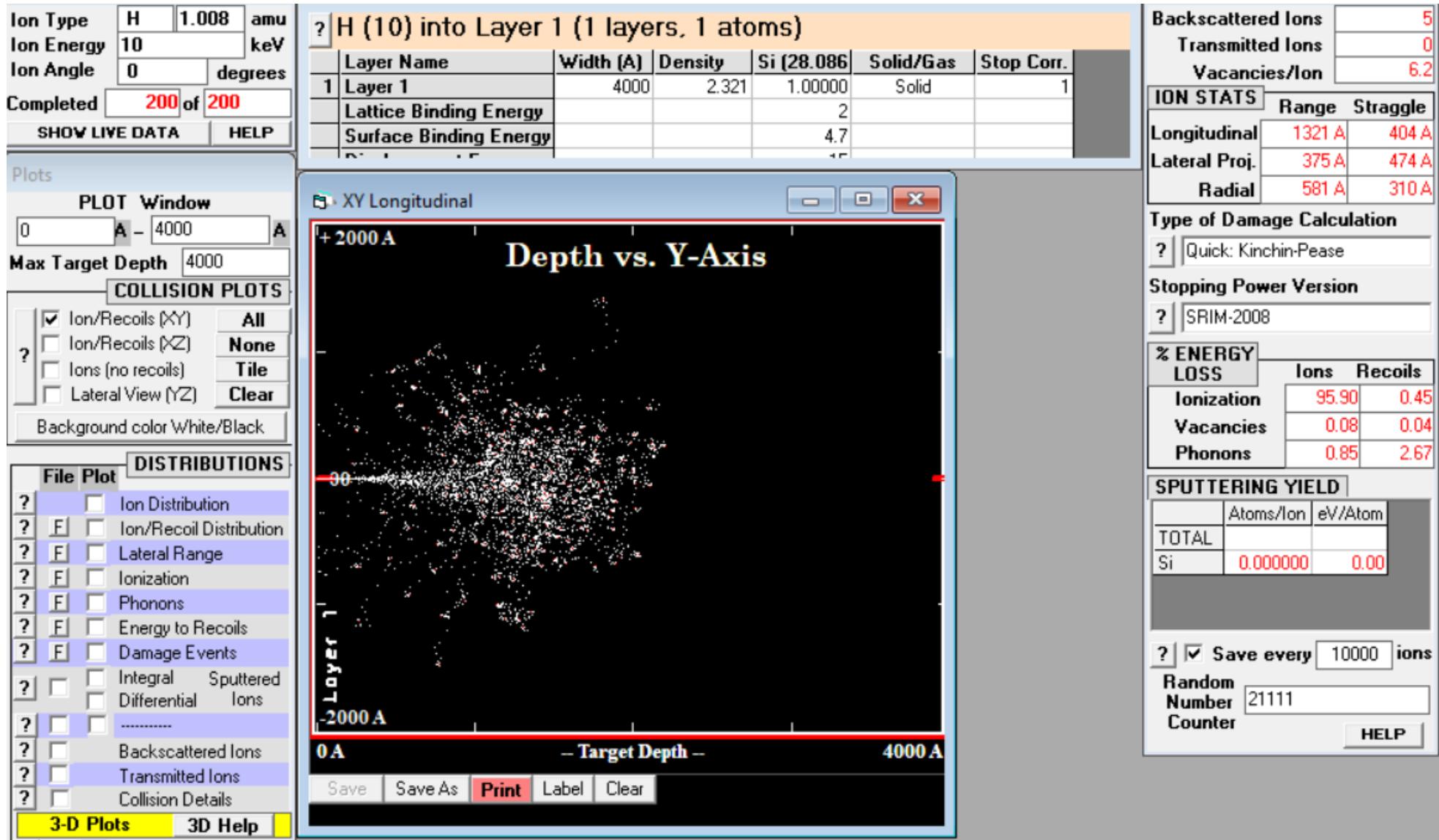
- Often also called TRIM due to the earlier name “Transport and Range of Ions in Matter”
- It can calculate any stopping power (electronic or nuclear) in any material, including compounds and multilayer one
- Includes electronic stopping in all calculations
- Downsides:
 - Only amorphous materials modelled => 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



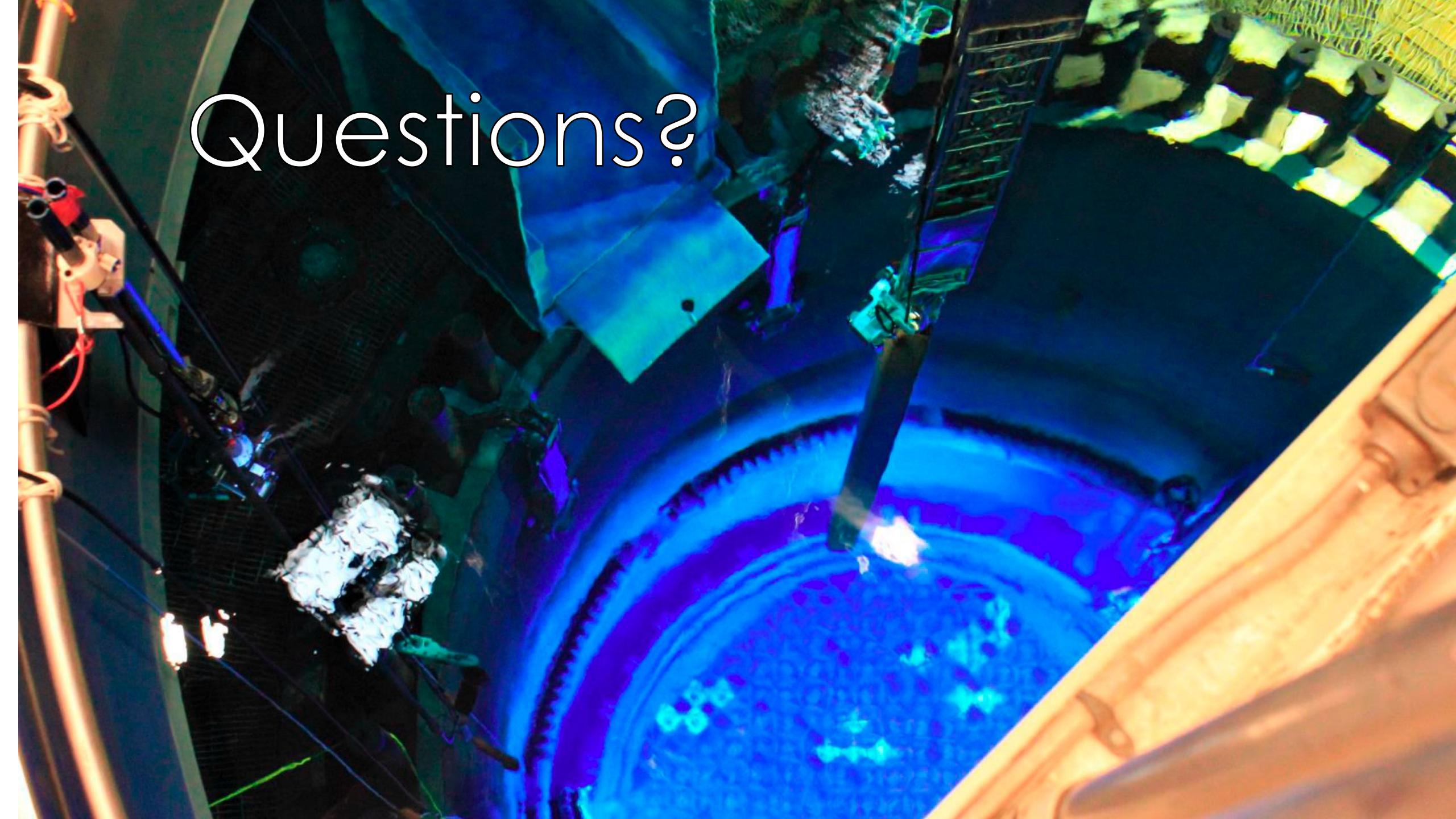
The SRIM software



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





Questions?