# *Atomic collisions, stopping of ions and defect production*

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1. ***Atomic collisions and energy loss mechanisms of high-energy ions***
2. ***Defect production and collision cascades***

***References:***

1. ***Chapter 17*** *of D. R. Olander,* *Fundamental Aspects of Nuclear Reactor Fuel Elements,* NTIS (1976)

# What is what?

***What is radiation:*** *Radiation: Radiation is the emission and transfer of energy through space!*

***What is radioactive material:*** *Any material that spontaneously emits any type of ionizing radiation.*

***What is radioactive contamination:*** *Radioactive material in an unwanted Location.*

***What is ionization:*** *The process of removing electrons from atoms to make charged ions.*

***What is dose:*** *The effect of radiation on mater.*

***What is an Isotope:*** *Any of the different forms of an element each having a different mass. Isotopes of an element have nuclei with the same number of protons (atomic number) but different number of neutrons.*

# What is dose?

***Counts per minute (cpm):*** *is a measure of radioactivity. It is the number of atoms in a given quantity of radioactive material that are detected to have decayed in one minute.*

***Becquerel (Bq):*** *is a measure for radioactivity. It is the disintegrations per second*

***Gray (Gy):*** *One gray is the absorption of one joule of radiation energy by one kilogram of matter.* ***J/kg***

***Sivert (Sv):*** *is the SI derived unit of dose equivalent. It attempts to reflect the biological effects of radiation as opposed to the physical aspects, which are characterized by the absorbed dose, measured in grays*

***Röntgen (roentgen)*** *equivalent in man or rem [rem] is a unit of radiation dose. It is the product of the absorbed dose in roentgens (R) and the biological efficiency of the radiation. 100 Rem equal 1 Sivert; the Sivert is the recommended SI derived unit,*

***Displacement per atom (dpa):*** *is a unit of radiation dose on materials.*

# Radiation damage in solids

- ***Radiation damage*** **refers to the localized disruption of the crystal lattice of a solid (defect production) by high-energy radiation passing through it.**

- ***Radiation effects*** **are the consequence of radiation damage on the mechanical and/or physical properties of the solid**

- **Solids consist of stationary atoms with:**
  - **a massive nucleus**
  - **electrons bound to the nucleus with energies ranging from keV (K-shell, heavy atoms) to eV (ionization potential of outer shell)**

- **Energetic particles of three types:**

  ***Neutral elementary particles***
  - **neutrons interact with atomic nuclei of solid atoms**
  - **gamma rays interact with electrons within the solid (pair production, compton scattering and photo-electric effect)**

  ***Charged elementary particles***
  - **protons, alpha particles**
  - **electrons (accelerator produced, beta particles & Compton)**

  ***High-energy atoms or ions***
  - **fission fragments**
  - **accelerator-produced heavy ions**
  - **recoil atoms (ions) of solid produced from primary collisions**

# *Interactions between energetic particles and solids*

- **Energetic charged particles interact independently with the nuclei and the electrons in a solid**
- **Interactions are characterized by *scattering cross sections***

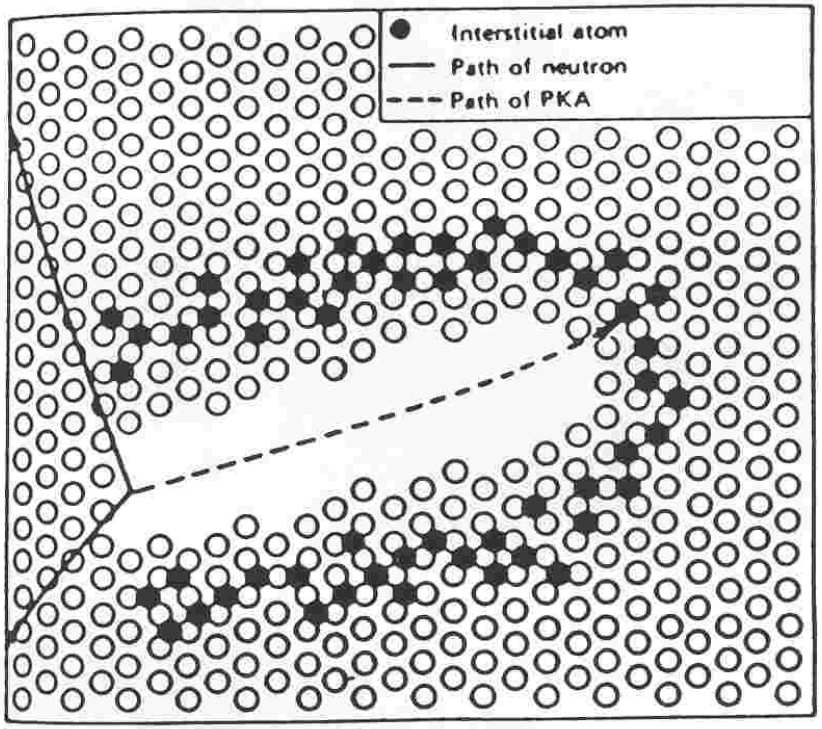
***Interactions between charged particles and electrons in a solid medium***

- **Characterized by the stopping power, or energy loss per unit path length**
- **Electronic stopping is dominant at high energies**
- **Electrons of the medium are excited (energized) and removed from the nucleus leading to ionization of the medium along ion-track**
- **Most of the energetic electrons are thermalized and re-captured by nuclei**
  **- Ionization energy is degraded into heat**
- **In insulators, some electrons are captured in defect sites, producing changes in electrical and magnetic properties**

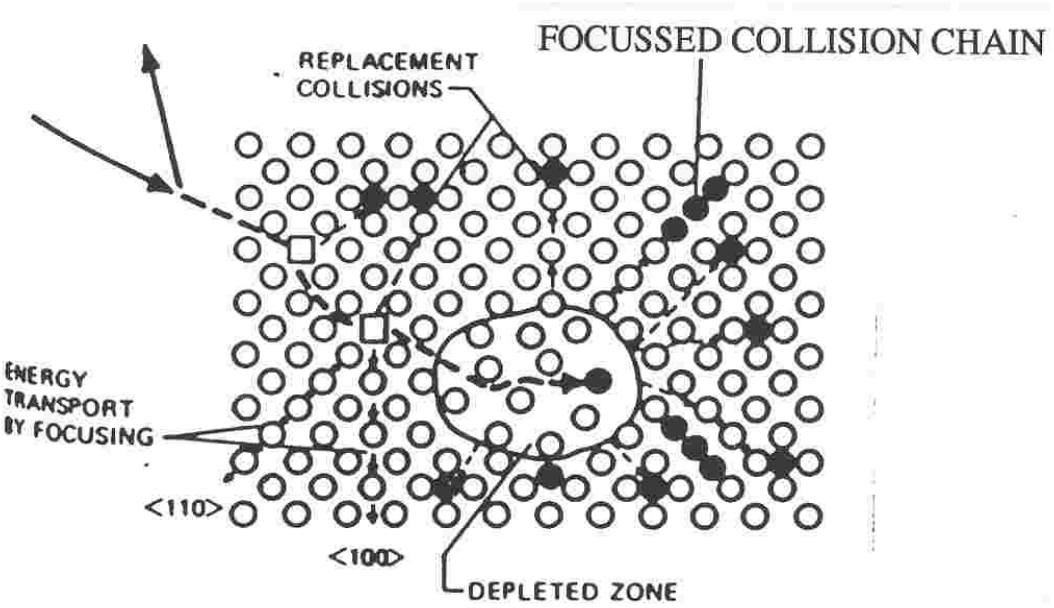
***Interactions between charged particles and nuclei in a solid medium***

- **Nuclear interactions predominate at low energies**
- **Nuclear interactions (scattering) involve:**
  **- bare nuclei at high particle energy**
  **- nuclei and bound electrons at low energies**
- **Nuclear interactions produce permanent atomic displacements within the solid**
- **Atomic displacements are the underlying cause of physical and mechanical property changes - *radiation damage* and *radiation effects***

# Displacement spike: *Early Qualitative Ideas*




Original model of the displacement spike, J.A. Brinkman, *Amer. J. Phys* 24 (1956) 24.




Later, but still qualitative, version of the displacement spike (also called depleted zone).

# There are ASTM standards!

Designation: E521 – 96 (Reapproved 2009)$^{\varepsilon 1}$

## Standard Practice for Neutron Radiation Damage Simulation by Charged-Particle Irradiation[1]

This standard is issued under the fixed designation E521; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon ($\varepsilon$) indicates an editorial change since the last revision or reapproval.

$\varepsilon^1$ NOTE—Editorial corrections were made in Section 14 in November 2012.

Designation: E798 – 96 (Reapproved 2009)

## Standard Practice for Conducting Irradiations at Accelerator-Based Neutron Sources[1]

This standard is issued under the fixed designation E798; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon ($\varepsilon$) indicates an editorial change since the last revision or reapproval.

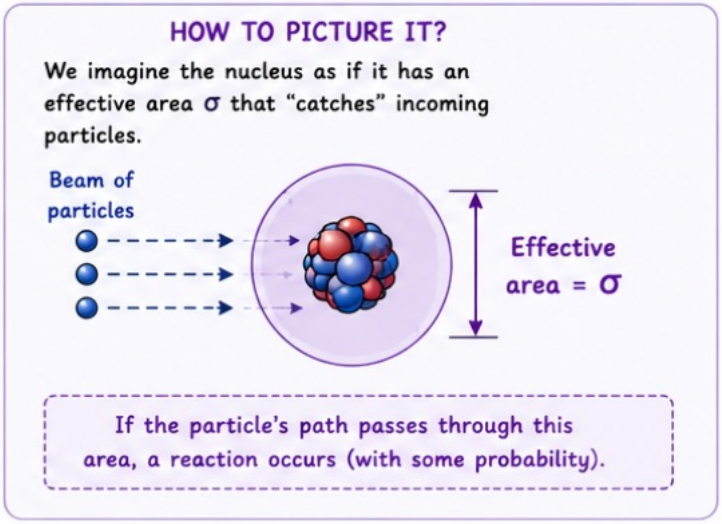
# # of interactions/reactions

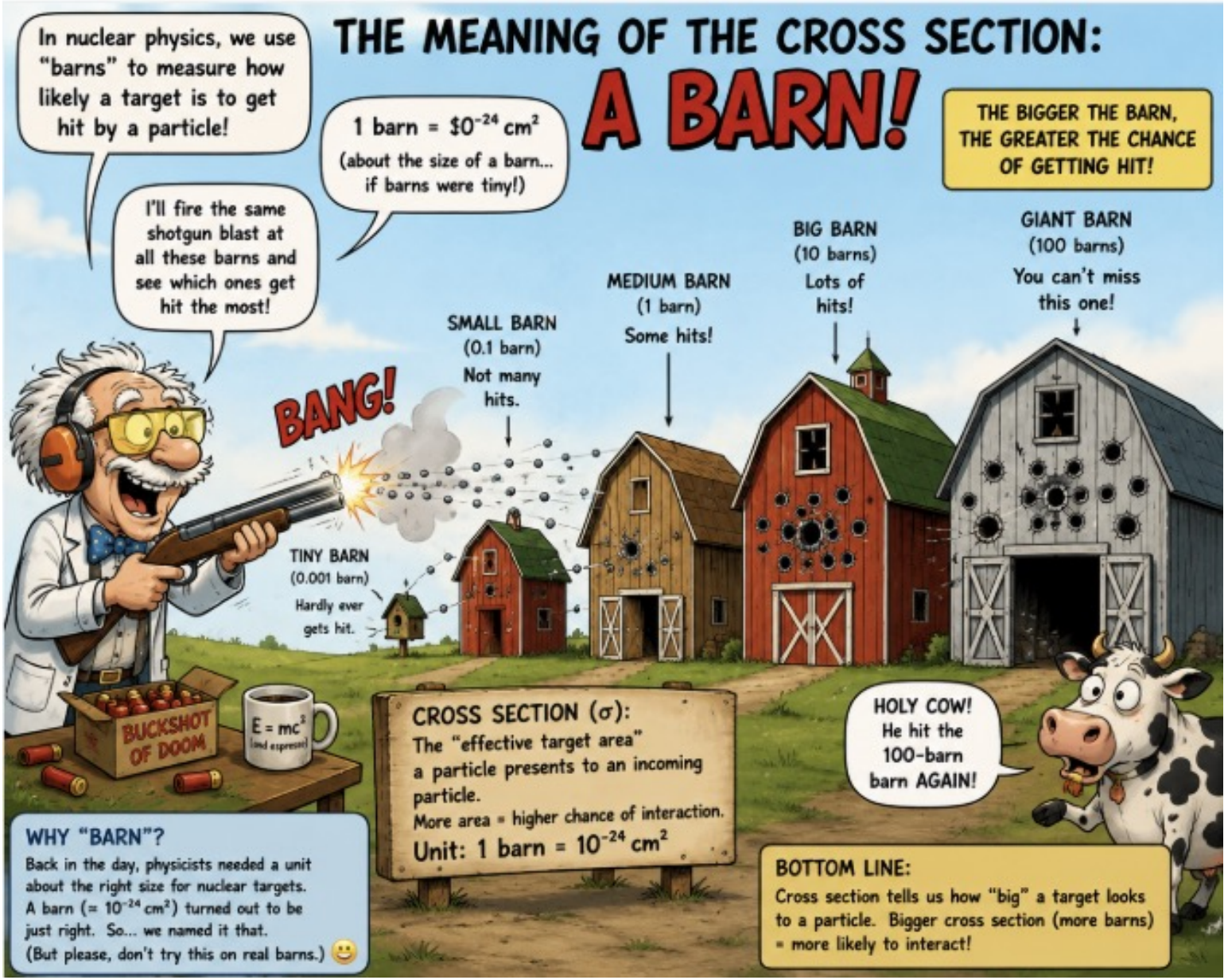
***The probability of a neutron fission is described by the nuclear cross section $\sigma$.***

$$r_x = \Phi\, \sigma_x\, \rho_A = \Phi \Sigma_x$$

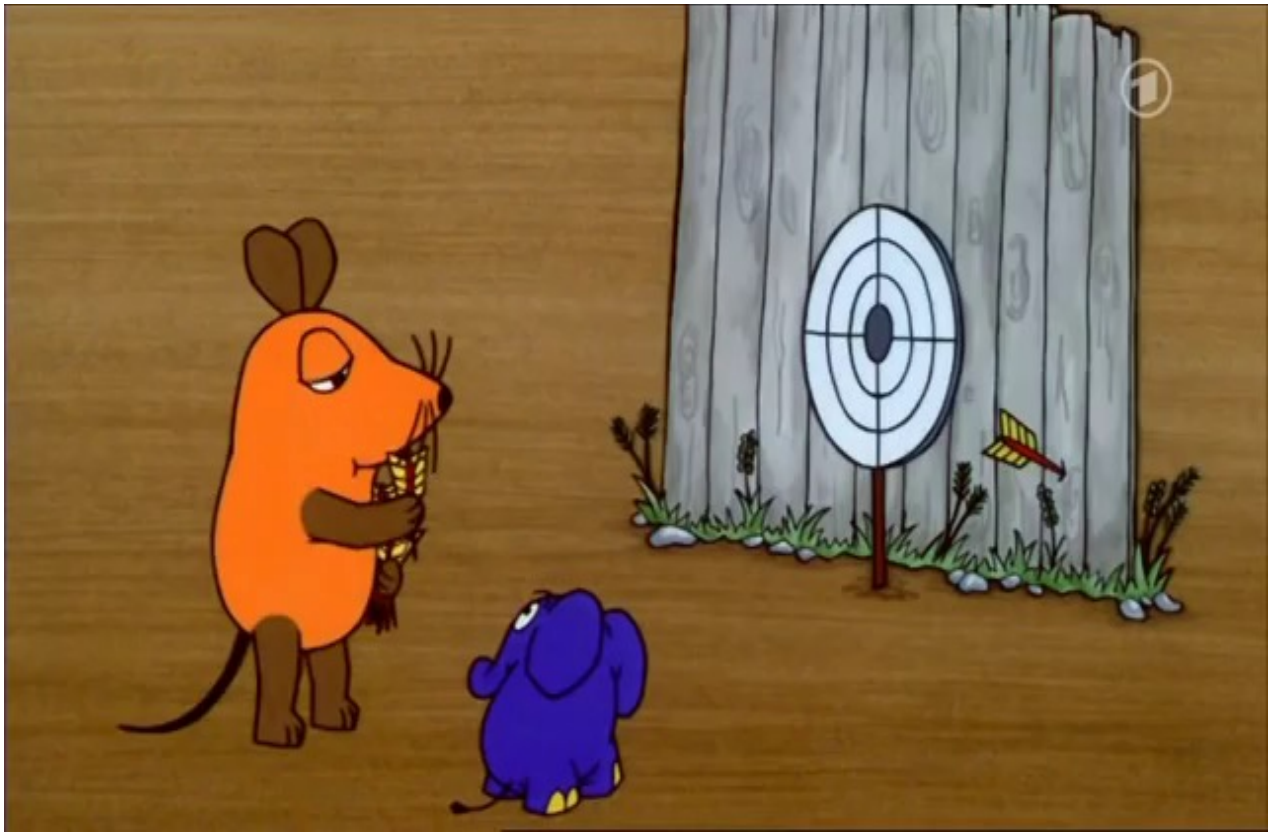
*Flux* — *Microscopic cross section* — density of atoms — *Macroscopic cross section*

***The nuclear cross section depends on the isotope and the energy of the incoming neutron***


THE MEANING OF THE CROSS SECTION:
A BARN!
In nuclear physics, we use "barns" to measure how likely a target is to get hit by a particle!
1 barn = $10^{-24}$ cm²
(about the size of a barn... if barns were tiny!)
I'll fire the same shotgun blast at all these barns and see which ones get hit the most!
THE BIGGER THE BARN, THE GREATER THE CHANCE OF GETTING HIT!
TINY BARN
(0.001 barn)
Hardly ever gets hit.
SMALL BARN
(0.1 barn)
Not many hits.
MEDIUM BARN
(1 barn)
Some hits!
BIG BARN
(10 barns)
Lots of hits!
GIANT BARN
(100 barns)
You can't miss this one!
BANG!
BUCKSHOT OF DOOM
E = mc²
CROSS SECTION (σ):
The "effective target area" a particle presents to an incoming particle.
More area = higher chance of interaction.
Unit: 1 barn = $10^{-24}$ cm²
HOLY COW! He hit the 100-barn barn AGAIN!
WHY "BARN"?
Back in the day, physicists needed a unit about the right size for nuclear targets. A barn (= $10^{-24}$ cm²) turned out to be just right. So... we named it that.
(But please, don't try this on real barns.)
BOTTOM LINE:
Cross section tells us how "big" a target looks to a particle. Bigger cross section (more barns) = more likely to interact!

# Cross section
# collision density



# Different types of cross sections

| Cross Section Type | Meaning |
|---|---|
| Total cross section | Probability of ANY interaction |
| Elastic scattering | Projectile bounces off nucleus |
| Inelastic scattering | Nucleus excited during collision |
| Absorption | Particle absorbed by nucleus |
| Capture | Particle absorbed without fission |
| Fission | Nucleus splits |
| Transfer / reaction | Nucleons transferred |
| Spallation | High-energy fragmentation |
| Fusion | Two nuclei combine |
| Charged particle reactions | Proton/alpha-induced reactions |
| Activation cross section | Produces radioactive isotope |

***Total Cross Section***

$$\sigma_T$$

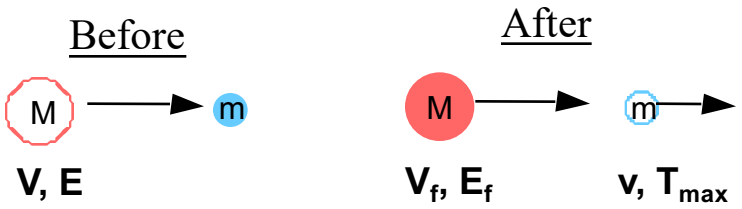
***Probability for ANY interaction to occur. Includes: scattering, absorption, fission , capture, reactions***

# Energy transfer in collisions

$$R = \frac{\text{collisions}}{\text{unit time} - \text{unit volume}} = N\sigma\phi \qquad (2.1)$$

N = atom density of solid (atoms/cm$^3$)
$\sigma$ = scattering cross-section (cm$^2$)
$\phi$ = flux of energetic particles (#/(cm$^2$-s))

***Head-on collision:***




M = mass of projectile particle
m = mass of struck atom
V, E = velocity, energy of projectile particle
v, $T_{max}$ = velocity, energy of struck particle after collision

***Conservation of energy in the head-on collision***

$$\frac{1}{2}MV^2 = \frac{1}{2}MV_f^2 + \frac{1}{2}mv^2 \quad \text{or} \quad E = E_f + T_{max}$$

***Conservation of linear momentum in the head-on collision***

$$MV = MV_f + mv \quad \text{or} \quad \sqrt{ME} = \sqrt{ME_f} + \sqrt{mT_{max}}$$

# Energy transfer in collisions

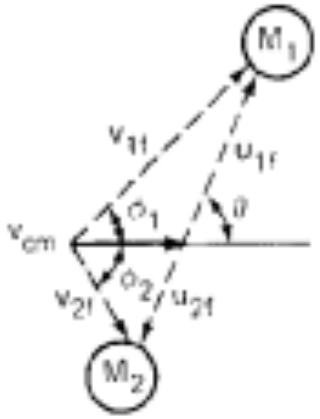
Solving simultaneously by eliminating $E_f$ yields the maximum energy transferred in the (head-on) collision:

$$T_{max} = \frac{4mM}{(m+M)^2} E = \Lambda E \qquad (2.2)$$

More generally, energy transferred to an atom in an elastic collision is given by:

$$T = \frac{1}{2} T_{max}(1-\cos\theta) = \frac{1}{2}\Lambda E(1-\cos\theta) \qquad (2.2a)$$

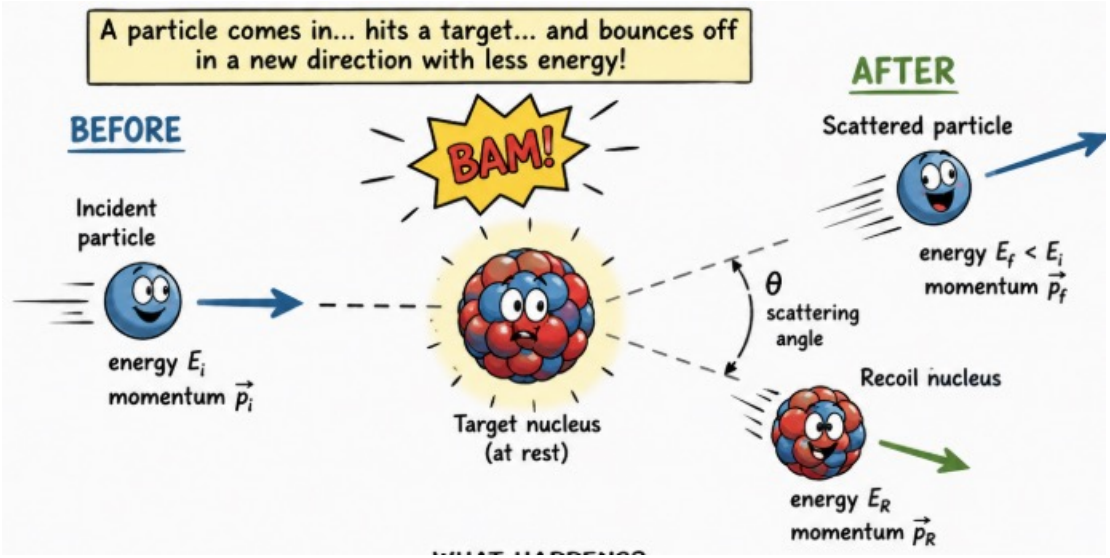
$\theta$ = center of mass scattering angle




- **In *hard-sphere* (billiard-ball) collisions, all values of T between 0 and $T_{max}$ are equally probable.**
- **The average energy transferred to the struck atom is $T_{max}/2$.**
- **Energy imparted to struck atoms causes displacements from the lattice sites in the crystal of the solid (*Frenkel pairs*) → *Radiation Damage***

# Energy transfer in collisions

**Example:** fission neutron collision with an iron atom

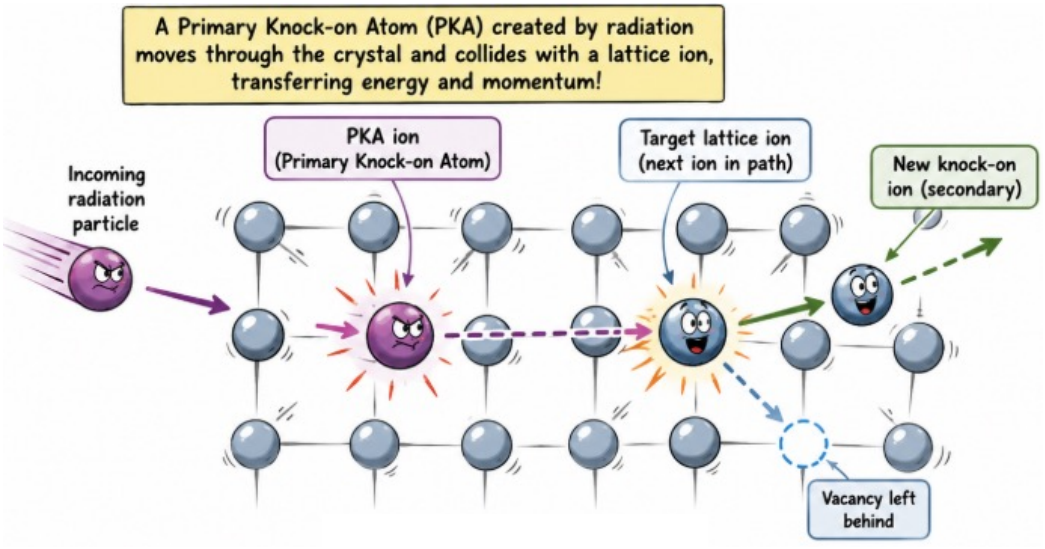



M = 1, E = 1 MeV (average energy of fission neutron); m = 56 (iron); Substituting into Eq. (2.2):

$$T_{max} = 0.07 \text{ MeV} = 70 \text{ keV} = 70{,}000 \text{ eV}$$

- The average energy of the first (iron) atom struck is 0.035 MeV = 35 keV = 35,000 eV; this struck atom is called the Primary Knockon Atom (**PKA**)

# Energy transfer in collisions




• Since about 25 eV ($E_d$ = *displacement energy*) is needed to displace a lattice atom from its site in the crystal, the PKA is displaced (often at high velocity), leaving behind a vacant lattice site

• The PKA strikes another lattice atom; since M = m (for atom - atom collisions), the average energy transferred to the second atom (Secondary Knockon Atom, SKA) is one-half of the PKA energy (17.5 keV)

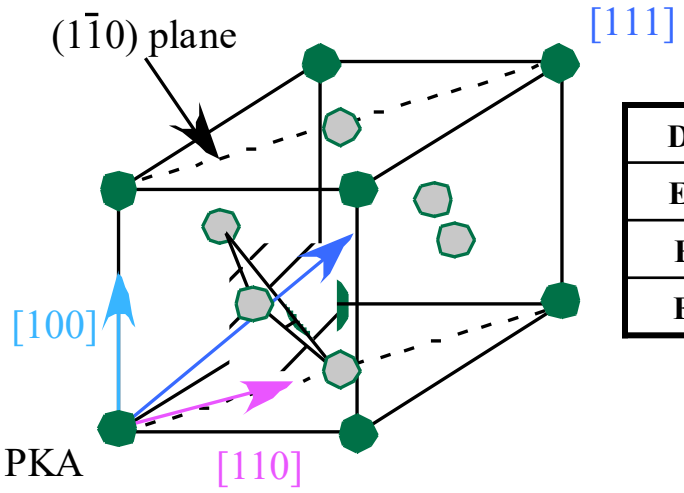
• The average energy of the recoils of the nth generation is one half of that of the previous generation. The process continues as a chain reaction until the recoil energy is less than $E_d \sim 25$ eV.

# Displacement Energy

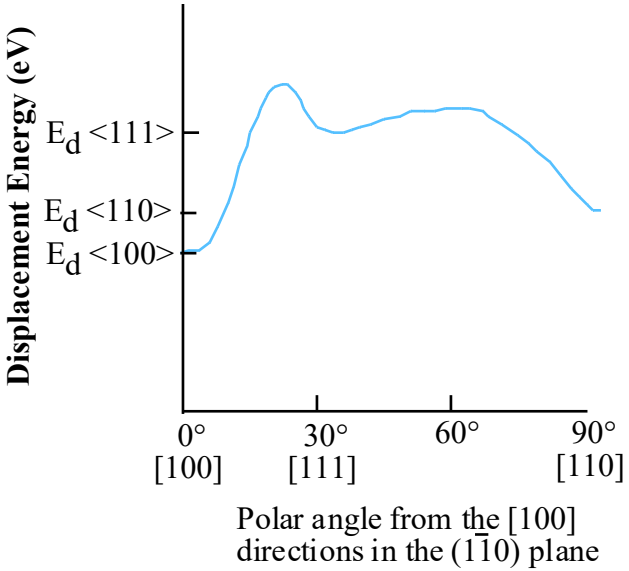
Because of the crystal structure of atoms in a solid, the displacement energy required to produce a Frenkel pair depends on PKA direction

- $E_d$ represents an average over all possible directions

Consider a face-centered cubic (fcc) crystal structure (Cu, Ni, stainless steel):



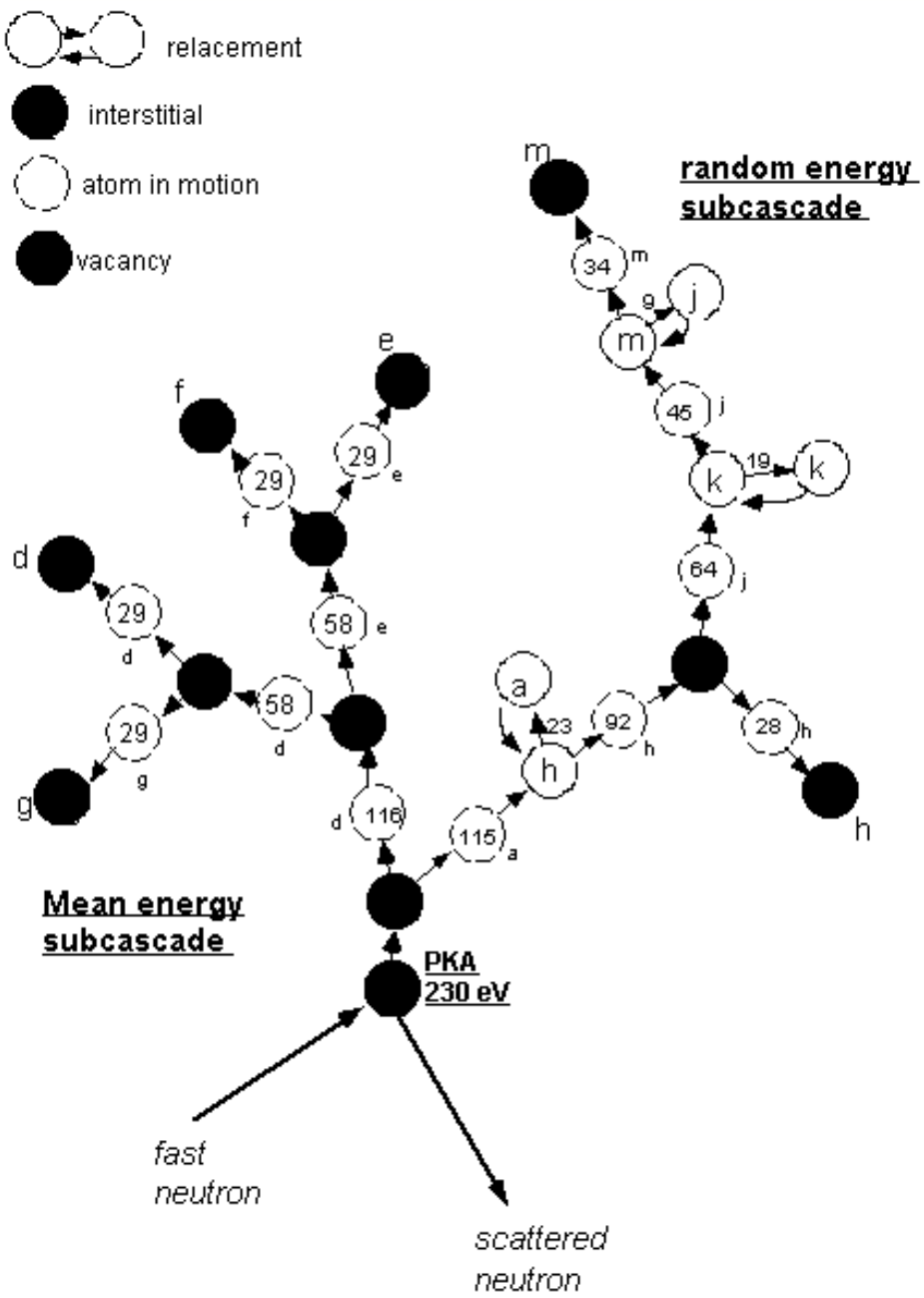

| Direction | Ref 1. | Ref 2. |
|---|---|---|
| $E_d$ <100> | 34 | 24 |
| $E_d$<111> | 43 | 80 |
| $E_d$<110> | - | 25 |

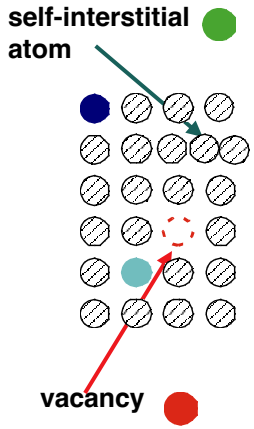



- **$E_d$ is much greater than the energy to create a V-SIA pair by equilibrium processes, since the collision is highly non-equilibrium.**
- **Average value of $E_d$ ~ 25 - 50 eV applies to most metals**


1. H.B. Huntington, *Phys Rev* **93** (1954) 1414.
2. J.B. Gibson, A.N. Goland, M. Milgram, G.H. Vineyard, *Phys Rev* **120** (1960) 1229.

# Example of cascade by low energy PKA's



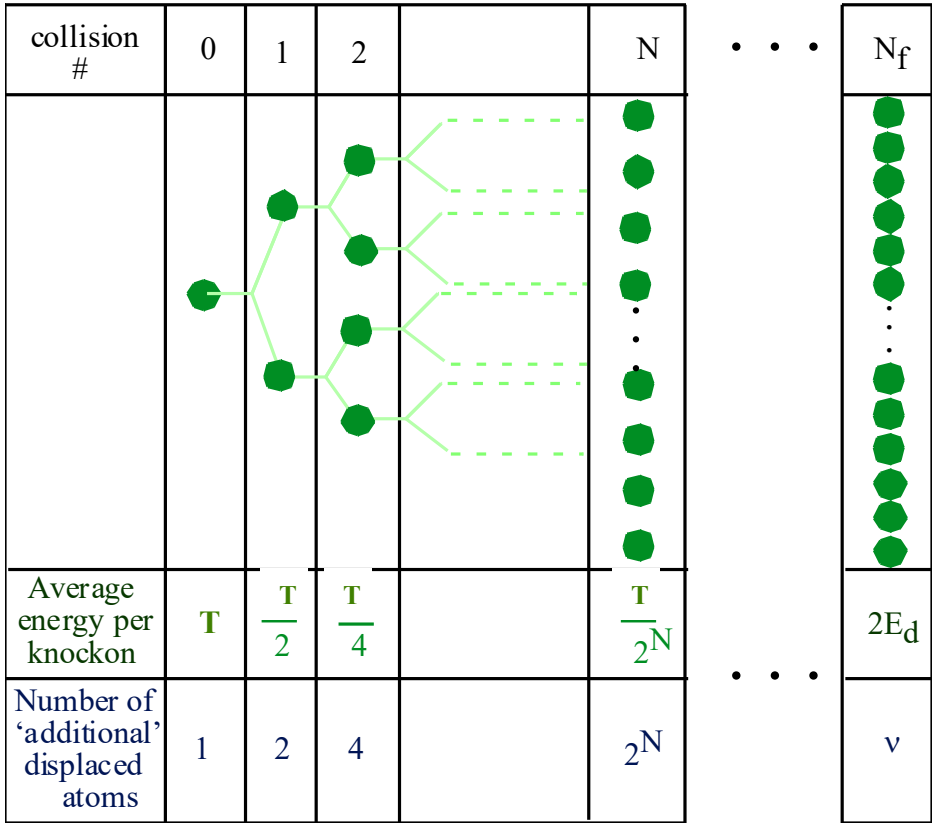

0.5 nm

# Lattice displacements due to a single PKA

- Thus, the single neutron initiates a collision cascade that contains n atomic displacements (*Frenkel pairs* or vacancy-(self)-interstitial pairs)

Because the PKA energy is so large compared to the displacement energy, each neutron generates many tens and even hundreds of V-I pairs

- $T \leq E_d$ - no displacements
- $E_d \leq T \leq 2E_d$ - only one PKA displaced ($T' < E_d$)
- For $T \geq 2E_d$




- Cascade ceases when average knockon energy is $2E_d = T/2^{Nf}$
- Final number of displaced atoms is $\nu = 2^{Nf}$

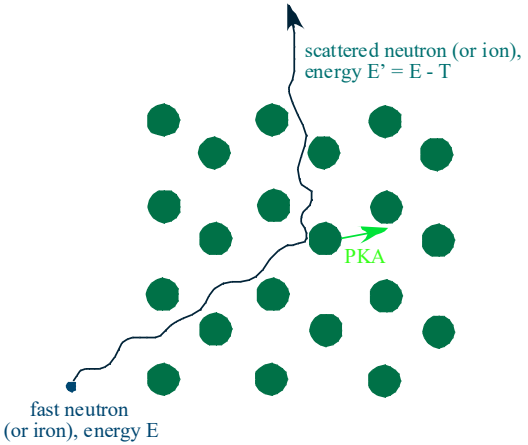
$$\nu = \frac{T}{2E_d} \qquad (2.3)$$

For iron example: $\nu = 35000/2/25 = 700$ displacements

# Number of displaced atoms from nuclear collisions

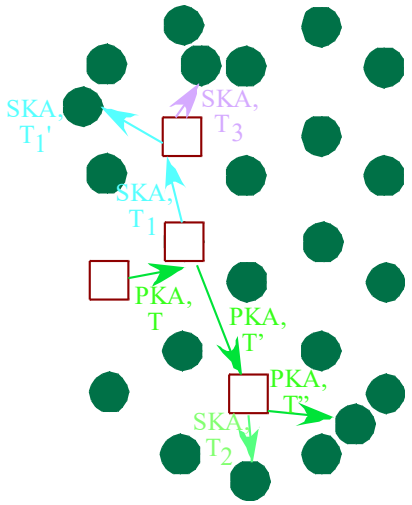
**A fast neutron (or ion) creates Primary Knockon Atoms (PKA) within a solid as a result of (primarily) elastic collisions with energy T.**

**Primary collision:**




**If $T > E_c$ - consider electronic energy loss (Bethe-Bohr or Lindhard) - no atomic displacements**

**For $T < E_c$ - consider atomic displacements (nuclear stopping) which produces vacancies and self-interstitial atoms**




**E = initial neutron energy**
**PKA = primary knockon atom = atom initially struck by energetic particle**
**SKA = secondary knockon atom**
**T (or E) = energy transferred to PKA**
**E' = neutron energy following collision**
**$T_j$ = energy transferred to struck atom j**
**$E_d$ = displacement energy = minimum energy transferred to lattice atom to produce permanent displacements (~ 25 eV)**
**$E_b$ = energy to form Frenkel (V + SIA) pair (~ 5eV)**

**Bombarding particles (material affected):**

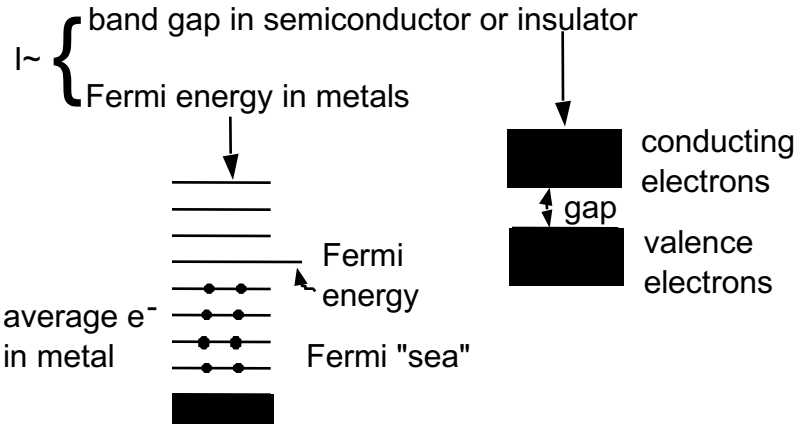
- **Fission fragments (fuel $UO_2$)**
- **fast neutrons (cladding, structures)**
- **$\alpha$-particles and protons (fusion reactor first wall)**
- **photons (structures - damage by Compton scattering)**
- **thermal neutrons:**

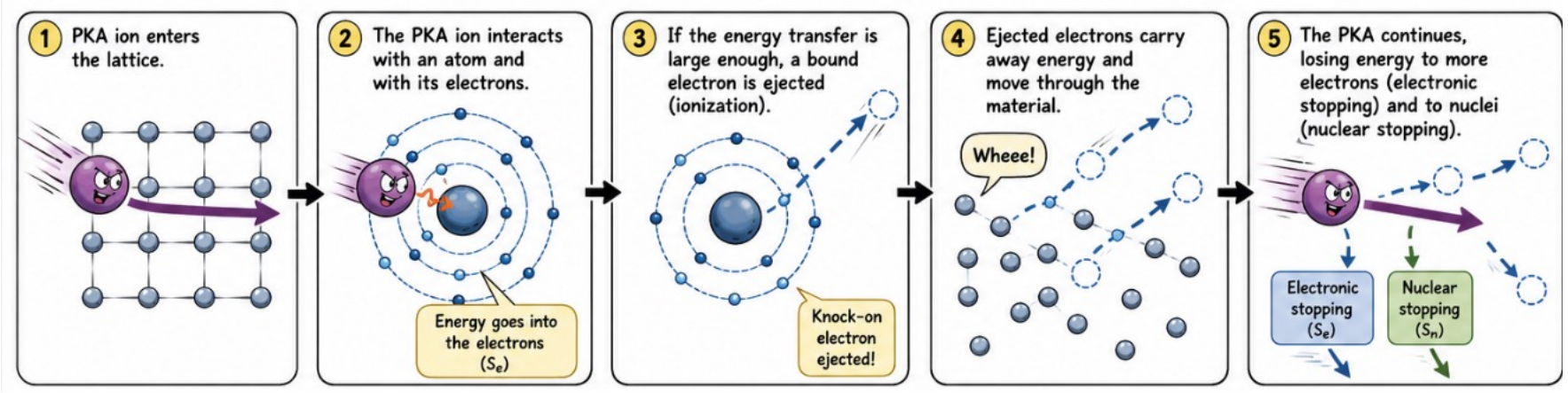
$$n + Fe^{56} \rightarrow Fe^{57} \xrightarrow{\gamma,\beta} Co^{57}$$

**Damage caused by recoil of $Co^{57}$ nucleus due to momentum transfer to $\gamma$**

# Energy loss to electrons (ionization of the solid)

- I = binding energy of electrons in medium (*like ionization potential*)



# Energy loss to electrons (ionization of the solid)

- In order for energy transfer from moving atom (or ion) to electron in medium to occur, a head-on collision of atom (or ion) and electron must transfer minimum energy I.

- From Eq. (2.2) with $T_{max} = I$, $m = m_e$, $E_c$ = minimum ion energy for transferring enough energy to an electron to remove it from the atom:

$$I = \frac{4m_eM}{(m_e + M)^2}E_c = \frac{4m_e}{M}E_c \quad \text{or} \quad E_c = \frac{M}{4m_e}I \qquad (2.11)$$

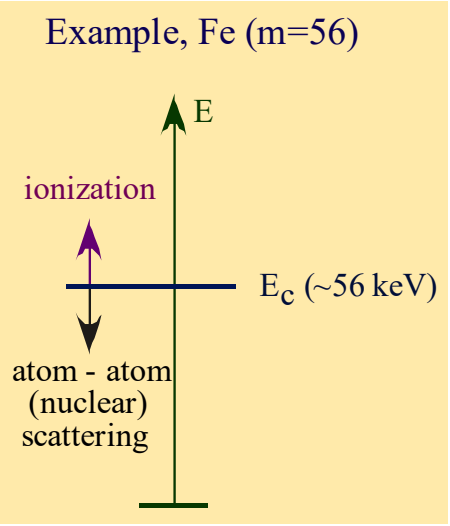
for I = 2 eV, $E_c = 10^3 M$ (eV)

- From the initial energy of the ion to $E_c$, the primary energy loss mechanism is *electronic stopping,* also simply called *ionization*

$$\left(\frac{dE}{dx}\right)_e = k\sqrt{E} = electronic\ stopping\ \ power\ of\ the\ medium; k = 8\sigma_e N\left(\frac{m_e}{M_1}\right)^{0.5}$$

**Simplified model of the interaction**

- for $E > E_c$, all energy loss is by ionization, no displacements
- for $E < E_c$, all energy loss by displacement collisions with atoms



# Calculation dpa in Fe for example

Iron example:

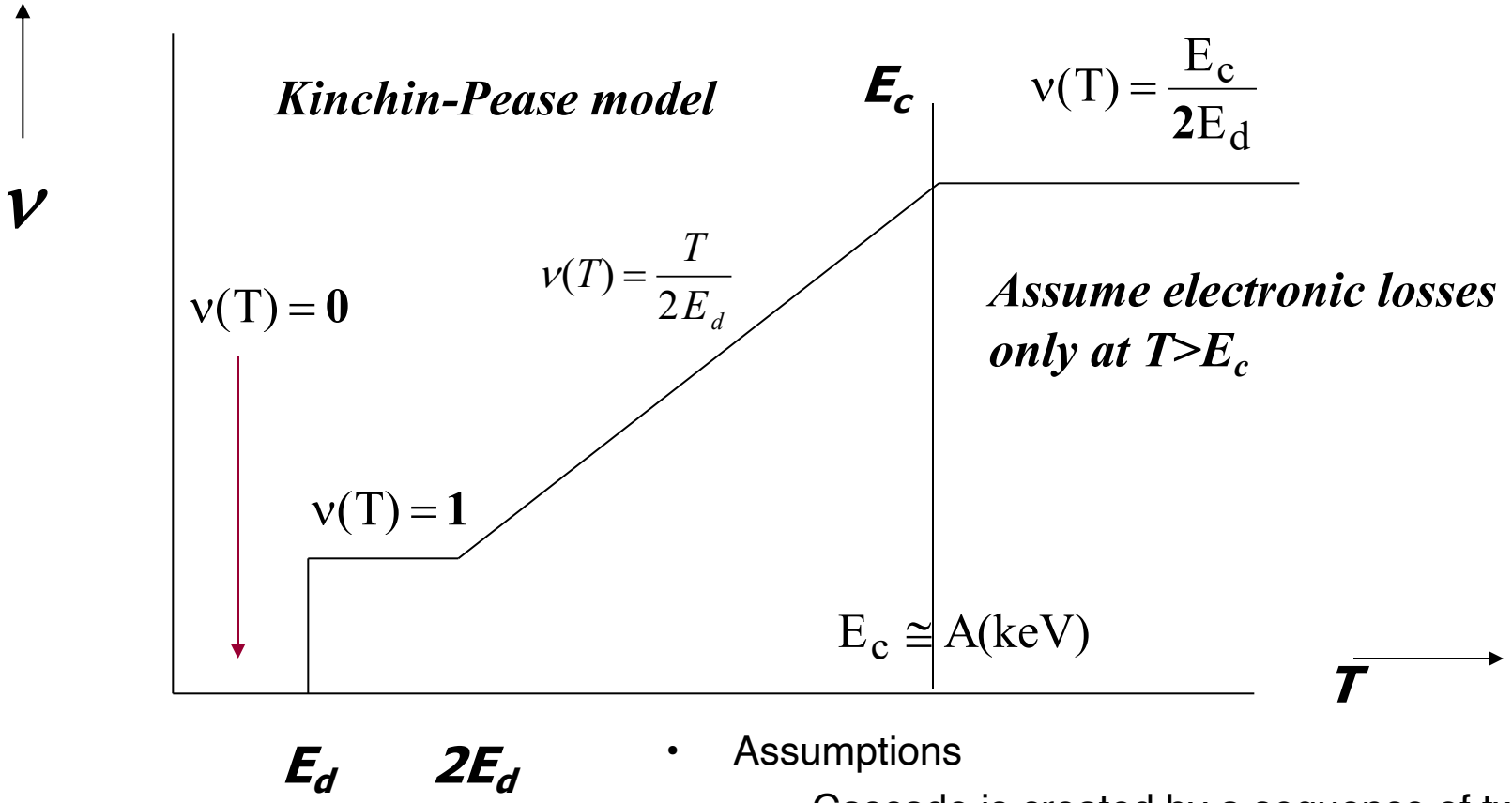
$\sigma$ = scattering cross section for 1 MeV neutrons ~ $3 \times 10^{-24}$ $cm^2$
N = atom density of iron atoms in solid ~ $8 \times 10^{22}$ atoms/$cm^3$
$\phi$ = fast neutron flux ~ $5 \times 10^{13}$ n/($cm^2$s)

- neutron - iron atom collision rate = $10^{13}$ collisions/$cm^3$/s
- displacement production rate = $(10^{13})(700) = 7 \times 10^{15}$ disp/$cm^3$/s (see earlier slide)
- in 3 years ($10^8$ s): $7 \times 10^{23}$ displacements/$cm^3$
- divide by atom density of iron to obtain "dose" in displacements per atom (dpa)

$$\text{dpa} = \frac{7 \times 10^{23}}{8 \times 10^{22}} \approx 9$$

Every atom is ripped off its lattice about 9 times!!

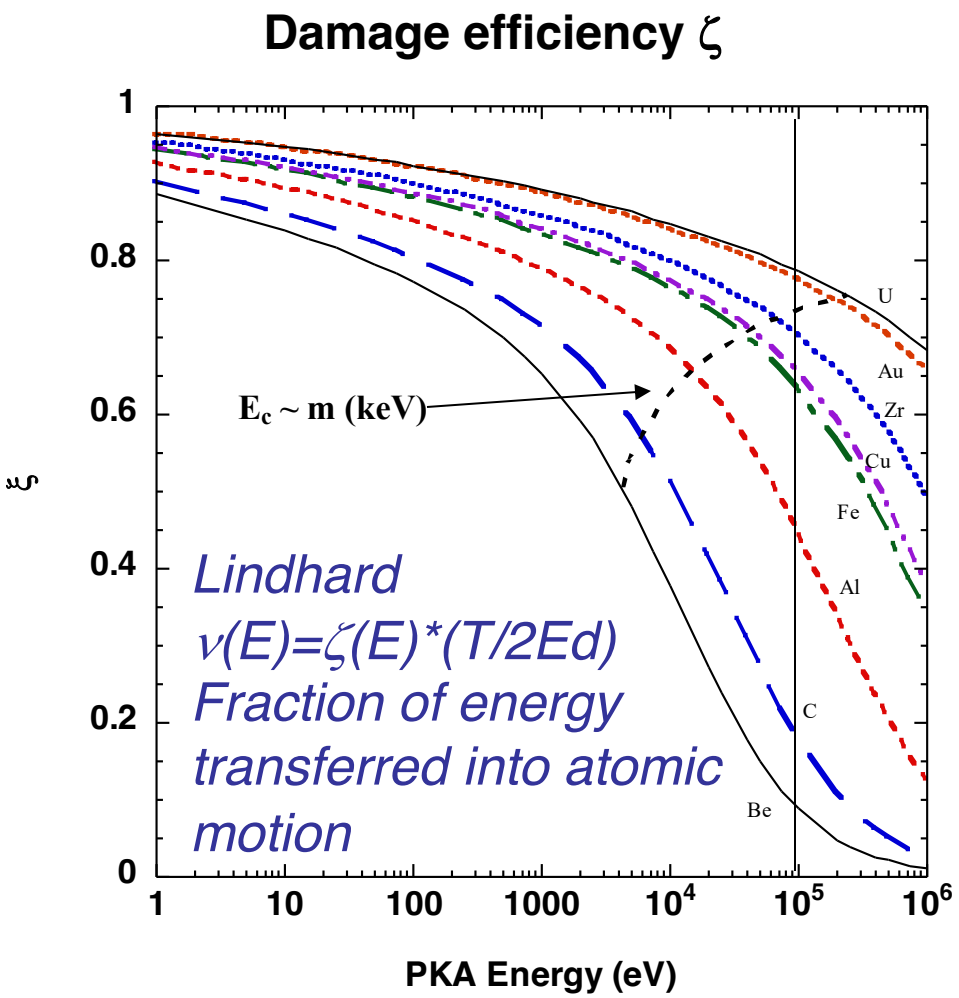
***Why doesn't the metal turn to powder???***

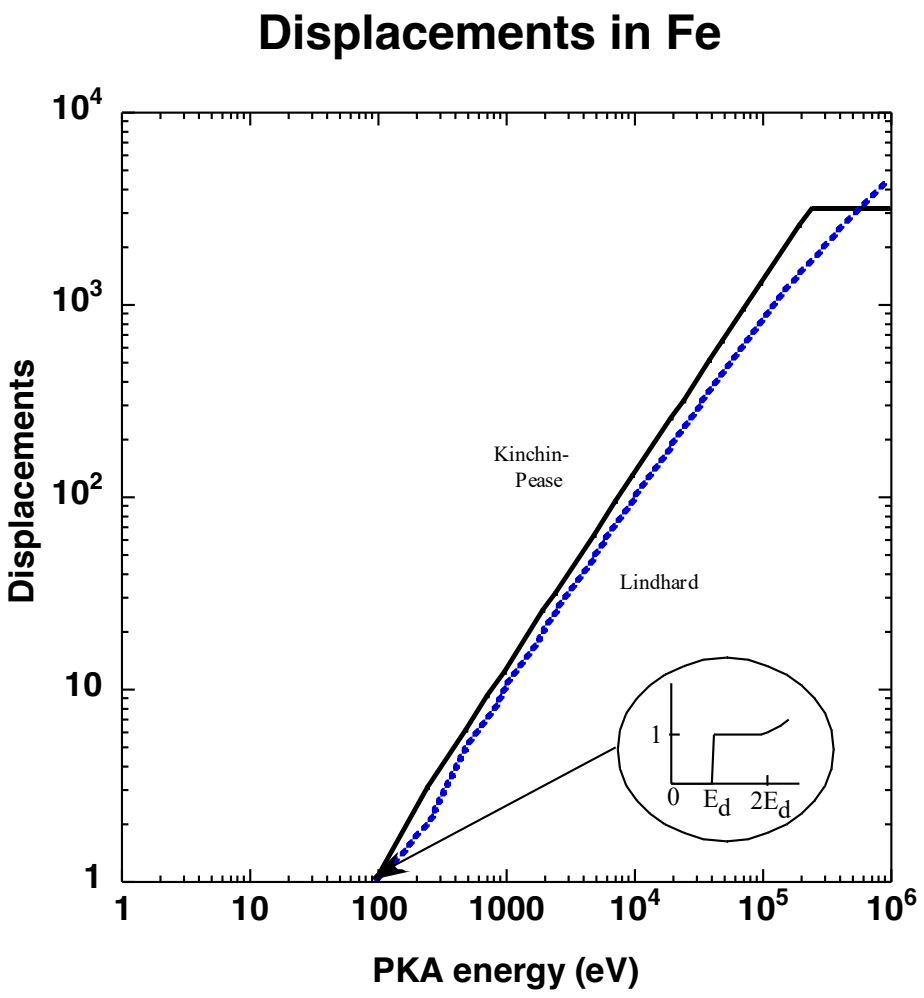



$$\nu(T) = \begin{cases} 0 & \text{for} \quad T < E_d \\ 1 & \text{for} \quad E_d < T < 2E_d \\ \dfrac{T}{2E_d} & \text{for} \quad 2E_d < T < Ec \\ \dfrac{E_c}{2E_d} & \text{for} \quad E_c < T \end{cases}$$

- Assumptions
  - Cascade is created by a sequence of two-body elastic collisions between atoms
  - The energy $E_d$ consumed in displacing an atom is neglected in the energy balance
  - Energy loss by electronic stopping is treated by a cutoff energy
  - Energy-transfer cross section is given by a hard-sphere model
  - The arrangement of atoms in the solid is random; effects due to crystal structure are neglected

# *Lindhard electronic energy loss*




***ζ= fraction of energy deposited in the material due to collision interaction***

# Norgett–Robinson–Torrens (NRT)

***KP- systematically overpredicted damage***

Detailed collision simulations showed that the KP equation predicted about 20–30% too many displaced atoms.

***Why?: Because real cascades are more complicated than ideal binary collisions.***

***For example:***

- *replacement collisions reduce the number of vacancies,*
- *energy is transferred to several atoms simultaneously,*
- *some recoil energy becomes lattice vibrations,*
- *not every collision splits energy exactly in half,*
- *some atoms receive just below* $E_d$.

***The Norgett–Robinson–Torrens (NRT) model first calculates the damage energy***

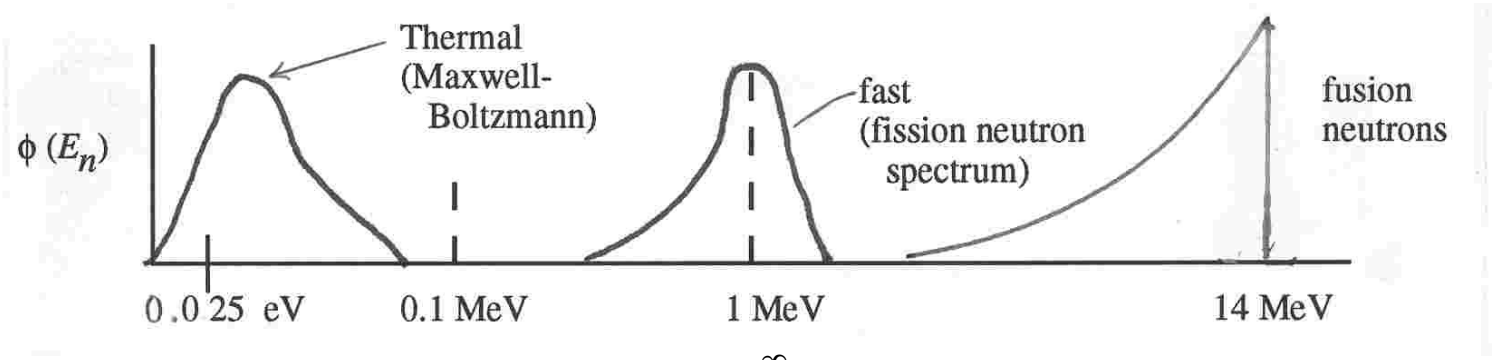
$$T_d$$

***after continuously subtracting electronic stopping using the Lindhard partition. Then***

$$N_d = 0.8 \frac{T_d}{2E_d}$$

# Fast neutron scattering & primary collision rate

- $E_n$ = neutron energy
  $\phi(E_n)dE_n$ = flux of neutrons with energies between $E_n$ and $E_n + dE_n$ (n/[cm$^2$-s-eV])




$$\Phi = \text{total fast flux} = \int_{0.1\text{MeV}}^{\infty} \phi(E_n)dE_n \quad \frac{\text{neutron}}{\text{cm}^2 - \text{s}} \qquad (2.4)$$

**Neutron scattering**

**n + lattice atom → PKA, energy T**

**$\sigma_n(E_n,T)$ = neutron differential energy transfer scattering cross section (elastic *and* inelastic)**

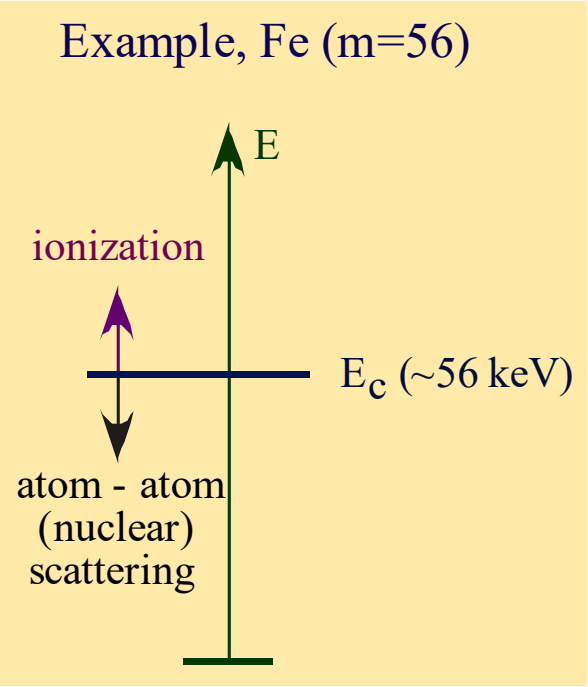
**The total neutron scattering cross section:**

$$\sigma_s(E_n) = \int_0^{\Lambda E_n} \sigma_n(E_n,T)dT$$

**For elastic scattering:**

$$T_{max} = \Lambda E_n \quad \overline{T} = \frac{1}{2}\Lambda E_n \quad \Lambda = \frac{4m}{(m+1)^2} \approx \frac{4}{m}$$

# Fast neutron interactions




**Fast reactor neutrons**

$$\bar{E}_n = 1 \quad \text{MeV}$$

$$\bar{T} = \frac{1}{2} T_{max}$$

$$\approx \frac{1}{2}\frac{4}{m}\bar{E}_n = \frac{2\bar{E}_n}{m} = \frac{2x1000}{56}(\text{keV})$$

$$\bar{T} \approx 36 \quad \text{keV}$$

**Fusion neutrons (14 MeV)**

$$\bar{T} = 500 \quad keV$$

## Displacement Cross Section

**Weight the differential scattering cross section with the number of displacements produced by the PKA of energy E:**

$$\sigma_d(E_n) = \int_{E_d}^{T_{max} = \Lambda E_n} \sigma_n(E_n, T)\nu(T)dT \qquad \textbf{(2.5)}$$

**For isotropic, elastic scattering:**

$$\sigma_n(E_n, T) = \frac{\sigma_s(E_n)}{\Lambda E_n} \qquad \textbf{(2.6)}$$

# Fast neutron interactions

**Approximate displacement function:**

$$\sigma_d = \frac{\sigma_s}{\Lambda E_n}\int_{E_d}^{T_{max}} \nu(T)dT = \frac{\sigma_s}{\Lambda E_n}\left[\int_0^{E_c}\left(\frac{T}{2E_d}\right)dT + \int_{E_c}^{\Lambda E_n}\left(\frac{E_c}{2E_d}\right)dT\right] = \left(\frac{E_c^2}{4\Lambda E_n E_d} + \frac{E_c(\Lambda E_n - E_c)}{2\Lambda E_n E_d}\right)\sigma_s \qquad \textbf{(2.7)}$$

**For iron: A (= m) = 56 ($\Lambda$ = 0.069);$E_d$ = 40 eV; $E_n$ = 1 MeV [fission neutrons]**

**$E_n$ = 14 MeV [fusion neutrons]**

**($E_c^2 + \Lambda E_n$ …) = 415 displaced atoms per neutron collision**

**($E_c^2 + \Lambda E_n$ …) = 680 displaced atoms per neutron collision**

**Using Equ above with $\sigma_s$ = 3 barns:**

**→ $\sigma_d$ ~ 1245 barns [fission] $\sigma_d$ ~ 2040 barns [fusion]**

**Relationship between number of displacements and Dose Rate**

***Displacement Rate:***

$$R_d = N\int_{E_d/\Lambda}^{\infty}\sigma_d(E_n)\phi(E_n)dE_n \qquad \frac{\text{displacements}}{\text{cm}^3 - \text{s}} \qquad \textbf{(2.8)}$$

**atom density (atoms/cm$^3$) = N = 1/$\Omega$ ($\Omega$ = atomic volume)**

$$K = \frac{R_d}{N} = \frac{\text{displacements}}{\text{atom} - \text{s}} = \int_{E_d/\Lambda}^{\infty}\sigma_d(E_n)\phi(E_n)dE_n = \frac{\text{dpa}}{\text{s}} \qquad \textbf{(2.9)}$$

# Fast neutron interactions - neutron displacement rate

**Approximation:**

**Evaluate $\sigma_d$ at $\overline{E}_n$= average neutron energy (> 0.1 MeV):**

$$K = \sigma_d \Phi \qquad (2.10)$$

**Example:**

**Fission neutrons** $\sigma_d \approx 1250$ barns $= 1.25 \times 10^{-21}$ cm$^2$
$\Phi \approx 5 \times 10^{13}$ n/(cm$^2$-s)

**in 5 yrs ~ $1.6 \times 10^8$ s, dpa = $(1.25 \times 10^{-21})(5 \times 10^{13})(1.6 \times 10^8) \approx 10$**

**Each atom in the solid is displaced 10 times in 5 years!!**

**For D-T fusion** $\sigma_d \approx 2040$ barns $\approx 2.0 \times 10^{-21}$ cm$^2$
$\Phi \approx 5 \times 10^{13}$ n/(cm$^2$-s)

**in 5 yrs ~ $1.6 \times 10^8$ s, dpa = $(2.0 \times 10^{-21})(5 \times 10^{13})(1.6 \times 10^8) \approx 16$**

**Each atom in the solid is displaced 16 times in 5 years (actually too low)**

**At high neutron energies**

- ***inelastic scattering*** **begins: n + m $\rightarrow$ m* + n'**
- ***anisotropic scattering*** **dominates: Eq. (2.6) is no longer applicable**
- **(n,p) and (n,$\alpha$) transmutations occur**

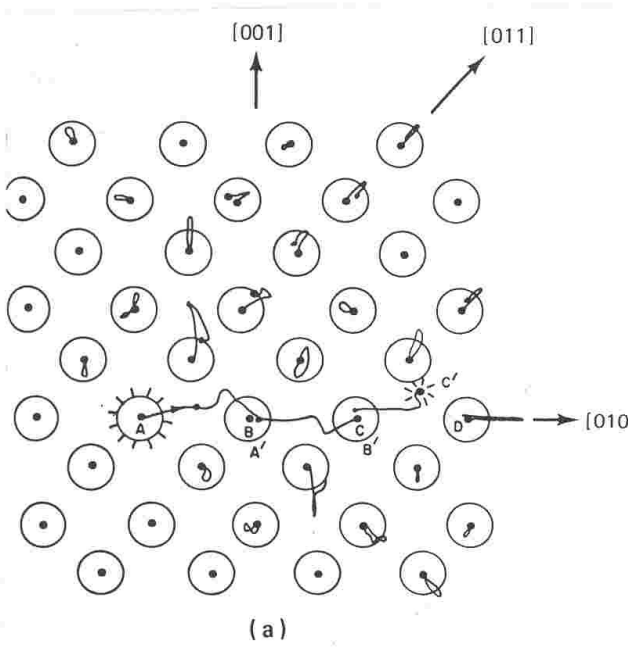
# Computer Simulation of Neutron Damage: Molecular Dynamics of Displacement Cascades

- A completely numerical representation of damage due to fast neutrons can be achieved by following the atomic trajectories in a crystallite of N lattice atoms, when one atom is given kinetic energy characteristic of a neutron scattering event
- The force on the $i^{th}$ atom in the crystal is the sum of forces from all neighboring atoms in the crystal, with Newton's 2nd law of motion applied to each atom (mass m):

$$m\frac{d^2\vec{x}_i}{dt^2} = \vec{F}_i = -\frac{\partial V(r_{i1}, r_{i2}, r_{ij} \ldots r_{iN})}{\partial \vec{r}_i} \qquad (2.12)$$

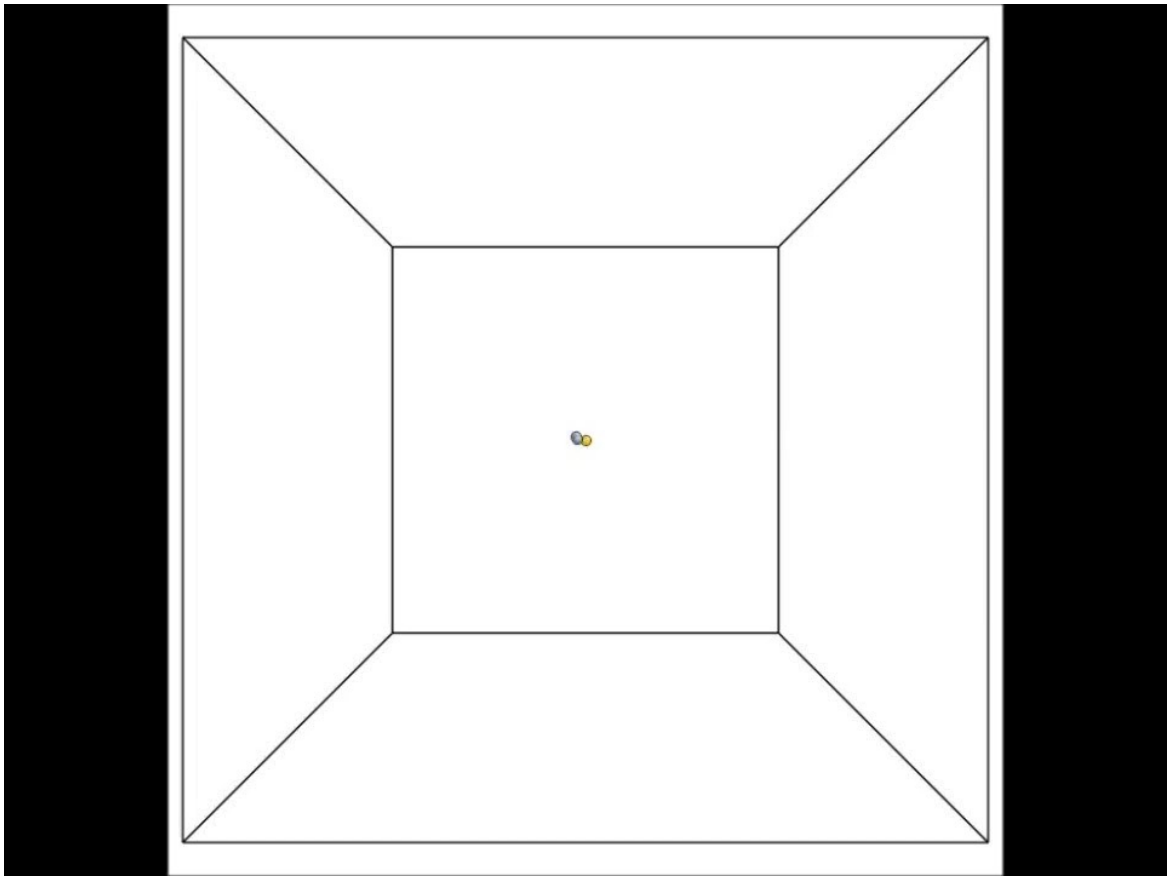
**$\vec{x}_i$ = position of the atom**
**$r_{ij}$ = separation between atoms i and j**
**$V(r_{ij})$ = potential energy between i-j pair**

- **The system of 3N (coupled) differential equations is solved for $\vec{x}_i$**
- **Note that the displacement energy, $E_d$, need not be specified a priori**
- **Shown to the right are early simulation results of a 40 eV PKA in the (100) plane of Cu**

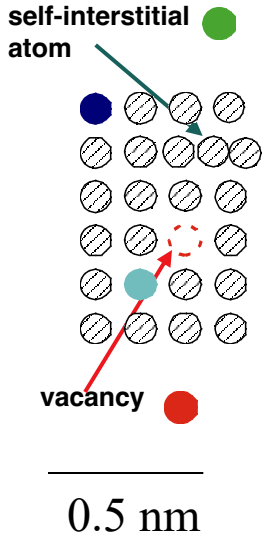


# Damage structure: high energy PKA

**Many atomic displacements (V-SIA) created at higher PKA energy and atomic displacement structure is clustered and spatially correlated (high energy PKAs typically result from heavy ion or fast neutron irradiation)**



**20 keV PKA in Fe:**
**the average energy transferred by a 550 keV neutron**



# Comparison of ion and fast neutron damage

**Since the energy transfer cross section for ions is an *atomic* cross section (~$10^{-17}$ $cm^2$) while that for neutrons is a *nuclear* cross section (~$10^{-24}$ $cm^2$),**

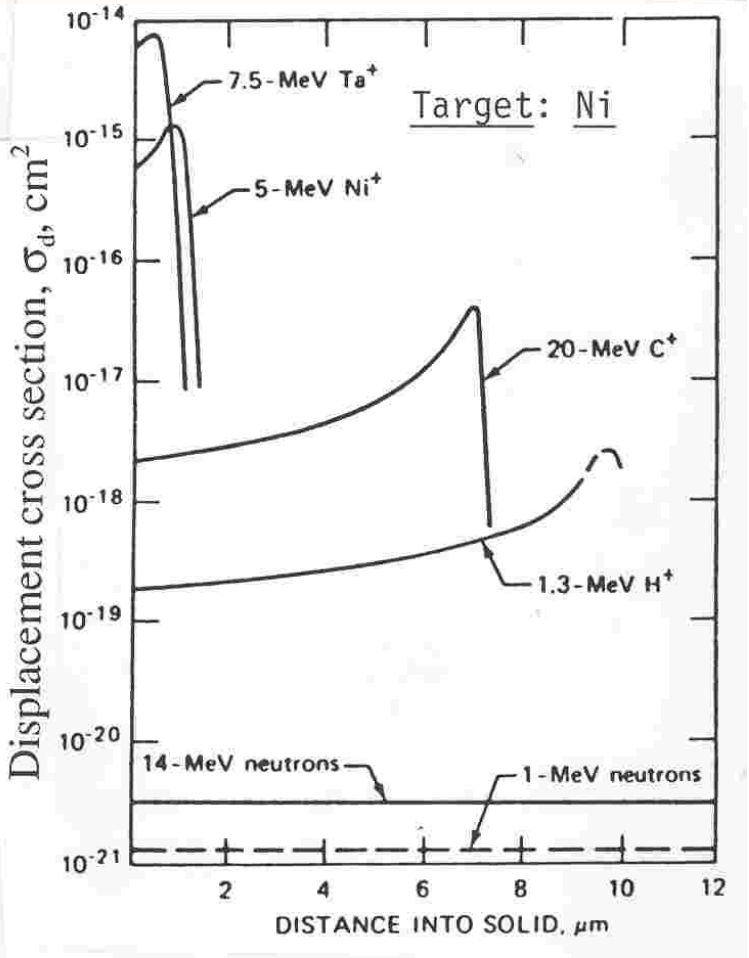
$(\sigma_d)_{ions} >> (\sigma_d)_{neutrons}$

**Examples:**

1) **20 MeV C+: I = $10^{14}$ $cm^{-2}sec^{-1}$ gives ~4x$10^{-3}$ dpa/s in a thin layer; dpa varies with penetration depth**

2) **neutrons give ~6x$10^{-8}$ dpa/s; dpa distribution is uniform**

| Characteristic | Neutrons | Ions |
|---|---|---|
| Flux, $cm^{-2}s^{-1}$ | 5x$10^{13}$ (isotropic) | $10^{11}$-$10^{12}$(beam) |
| dose rate, dpa/s | ~ $10^{-7}$ | $10^{-5}$ - $10^{-4}$ |
| Time for 1 dpa | ~ 4 mo. | 3 - 30 hr |
| Temp., °C | ~ 300 | adjustable |
| Macro. damage distr. | uniform | peak at end of range |
| Micro. damage distr. | inhomogeneous | inhomogeneous |
| Irradiated area | large | ~ 1 $cm^2$ |
| Irradiation depth | bulk | 1 - 10 μm nr. Surf. |
| Free defect fraction | 3 - 10% | ~ 30% |
| $\sigma_d$ , $cm^2$ | ~ $10^{-21}$ Eq(1.52) | $10^{-18}$-$10^{-15}$ Eq(1.89) |

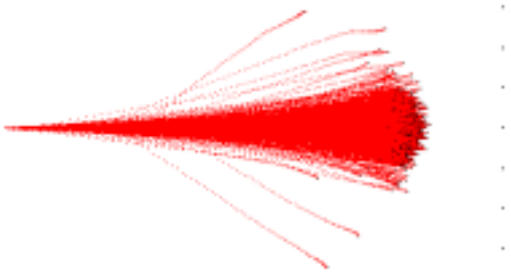


# SRIM *The Stopping and Range of Ions in Matter*

SRIM is a group of programs which calculate the stopping and range of ions (up to 2 GeV/amu) into matter using a quantum mechanical treatment of ion-atom collisions

SRIM is a Kinetic Monte-Carlo program (so no time dependence)that uses the potentials you've talked about in class to simulate radiation damage in a material

***Calculates most aspects of the energy loss of ions in matter, produces tables of stopping powers, range and straggling distributions for any, ion at any energy in any elemental target and is able to do targets with complex multi-layer configurations***



# SRIM *INPUT*

Material composition ; Material configuration (SRIM can handle layers of differing composition)
Displacement energy of each element in each layer for every material
SRIM will recommend a displacement energy
Density of each layer of material; SRIM can calculate this for you – not necessarily accurate
Incident ion type and energy
Type of calculation

***Types of SRIM calc:***

***Ion Distribution and Quick Calculation of Damage***

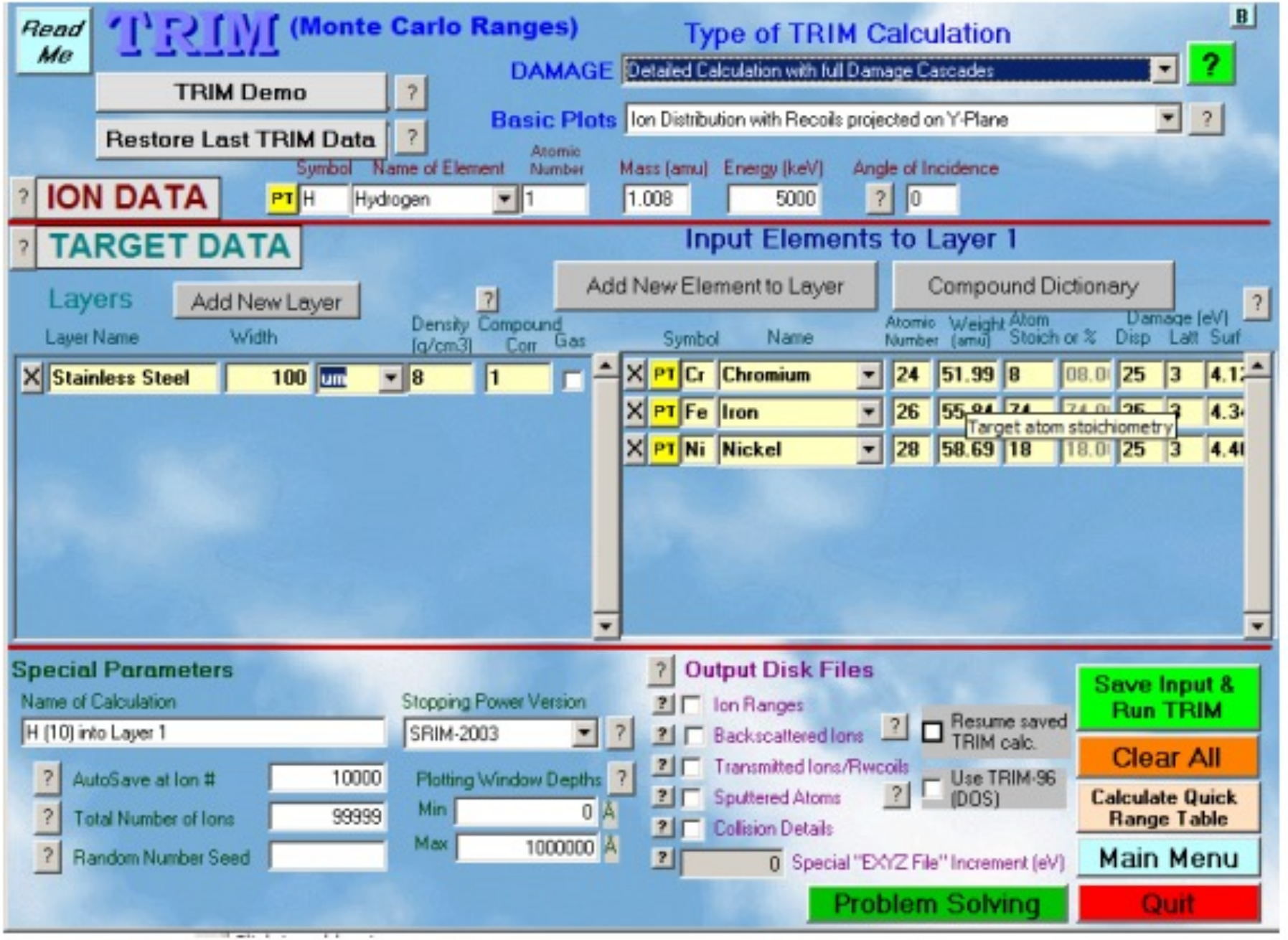
Don't care about details of target damage or sputtering; Quick statistical estimates based on the Kinchin-Pease Model

***Detailed Calculation with full Damage Cascades***

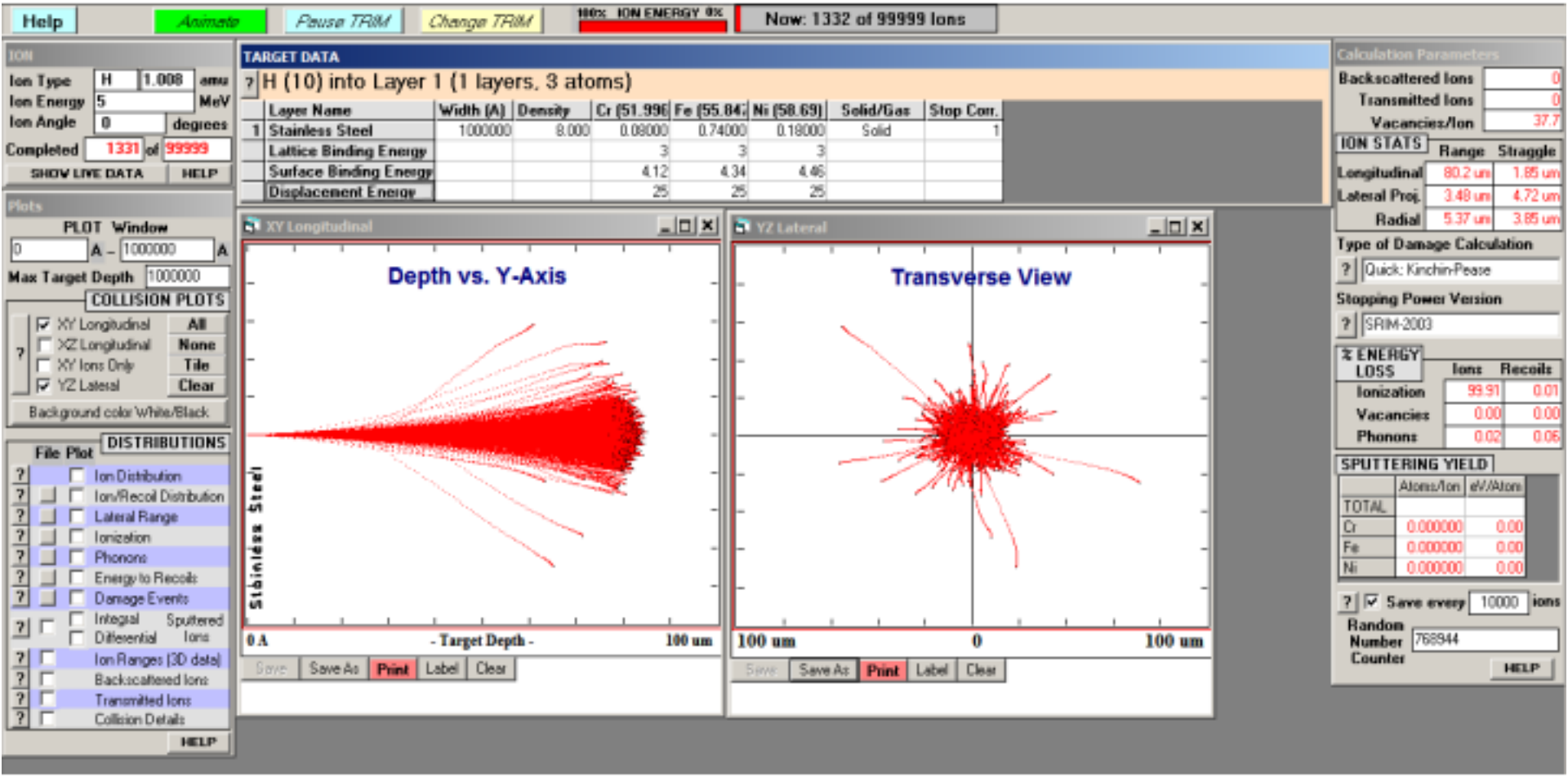
Follows every recoil until its energy drops below the lowest displacement energy of any target atom; All collision damage to the target is analyzed.

***Surface Sputtering / Monolayer Collisions***

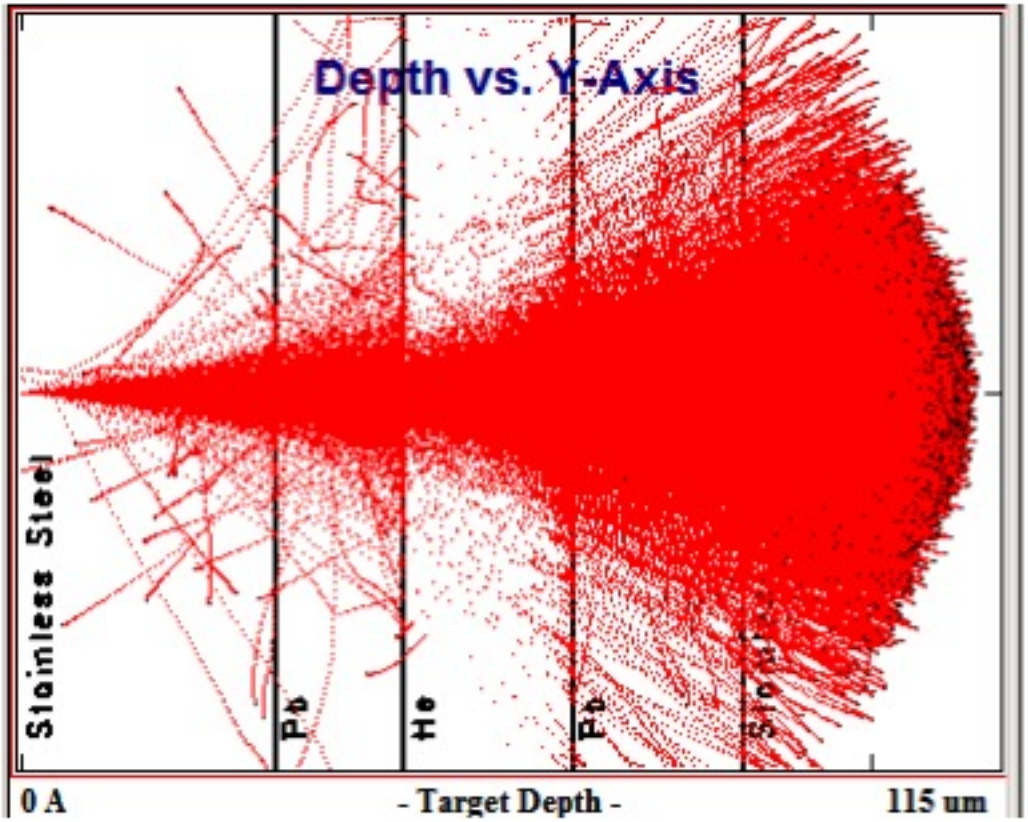
A full treatment of sputtering is contained in the above calculation for full damage cascades. ***TRIM contains the concept of a "free flight path", in which ions make large jumps between collisions and any target damage is spread over the jumped target atoms.***

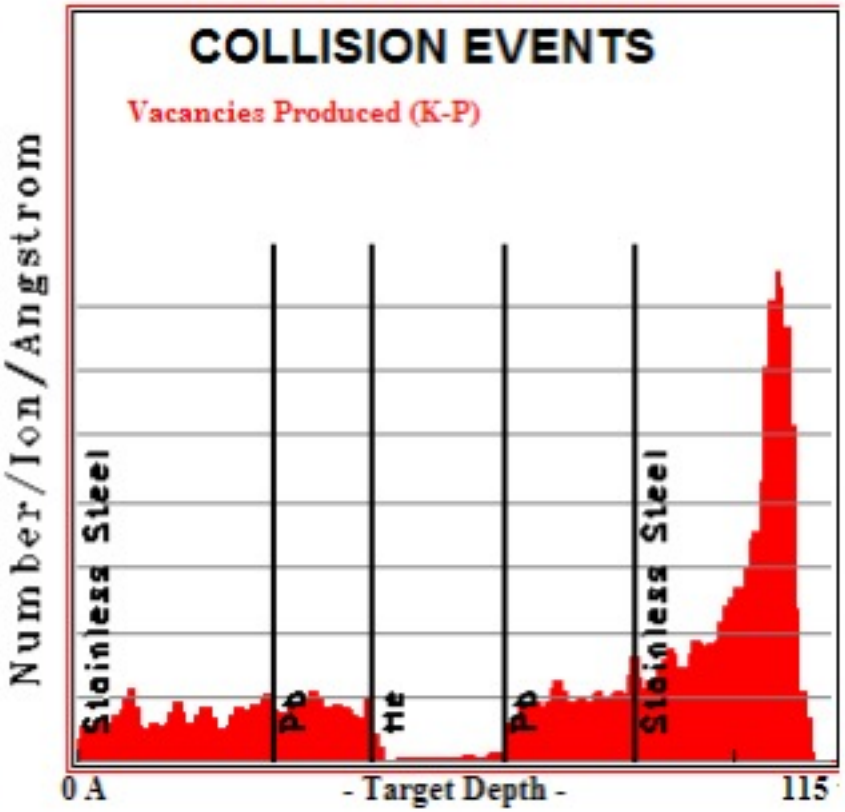

Read Me
TRIM (Monte Carlo Ranges)
Type of TRIM Calculation
DAMAGE
Detailed Calculation with full Damage Cascades
TRIM Demo
Restore Last TRIM Data
Basic Plots
Ion Distribution with Recoils projected on Y-Plane
ION DATA
Symbol
Name of Element
Atomic Number
Mass (amu)
Energy (keV)
Angle of Incidence
PT
H
Hydrogen
1
1.008
5000
0
TARGET DATA
Input Elements to Layer 1
Layers
Add New Layer
Add New Element to Layer
Compound Dictionary
Layer Name
Width
Density [g/cm3]
Compound Corr
Gas
Stainless Steel
100
um
8
1
Symbol
Name
Atomic Number
Weight (amu)
Atom Stoich or %
Damage [eV] Disp
Latt
Surf
Cr
Chromium
24
51.99
8
25
3
Fe
Iron
26
55.84
74
25
3
Ni
Nickel
28
58.69
18
25
3
Target atom stoichiometry
Special Parameters
Name of Calculation
H (10) into Layer 1
Stopping Power Version
SRIM-2003
AutoSave at Ion #
10000
Total Number of Ions
99999
Random Number Seed
Plotting Window Depths
Min
0
Å
Max
1000000
Å
Output Disk Files
Ion Ranges
Backscattered Ions
Transmitted Ions/Recoils
Sputtered Atoms
Collision Details
Special "EXYZ File" Increment (eV)
0
Resume saved TRIM calc.
Use TRIM-96 (DOS)
Save Input & Run TRIM
Clear All
Calculate Quick Range Table
Main Menu
Problem Solving
Quit

# SRIM *Output*


Help
Animate
Pause TRIM
Change TRIM
100% ION ENERGY 0%
Now: 1332 of 99999 Ions
ION
Ion Type H 1.008 amu
Ion Energy 5 MeV
Ion Angle 0 degrees
Completed 1331 of 99999
SHOW LIVE DATA
HELP
Plots
PLOT Window
0 A – 1000000 A
Max Target Depth 1000000
COLLISION PLOTS
XY Longitudinal
XZ Longitudinal
XY Ions Only
YZ Lateral
All
None
Tile
Clear
Background color White/Black
DISTRIBUTIONS
File Plot
Ion Distribution
Ion/Recoil Distribution
Lateral Range
Ionization
Phonons
Energy to Recoils
Damage Events
Integral
Differential
Sputtered Ions
Ion Ranges (3D data)
Backscattered Ions
Transmitted Ions
Collision Details
HELP
TARGET DATA
H (10) into Layer 1 (1 layers, 3 atoms)
Layer Name | Width (A) | Density | Cr (51.996) | Fe (55.847) | Ni (58.69) | Solid/Gas | Stop Corr.
1 Stainless Steel | 1000000 | 8.000 | 0.08000 | 0.74000 | 0.18000 | Solid | 1
Lattice Binding Energy | 3 | 3 | 3
Surface Binding Energy | 4.12 | 4.34 | 4.46
Displacement Energy | 25 | 25 | 25
XY Longitudinal
Depth vs. Y-Axis
Stainless Steel
0 A
- Target Depth -
100 um
Save
Save As
Print
Label
Clear
YZ Lateral
Transverse View
100 um
0
100 um
Save
Save As
Print
Label
Clear
Calculation Parameters
Backscattered Ions 0
Transmitted Ions 0
Vacancies/Ion 37.7
ION STATS
Range
Straggle
Longitudinal 80.2 um 1.85 um
Lateral Proj. 3.48 um 4.72 um
Radial 5.37 um 3.85 um
Type of Damage Calculation
Quick: Kinchin-Pease
Stopping Power Version
SRIM-2003
% ENERGY LOSS
Ions
Recoils
Ionization 99.91 0.01
Vacancies 0.00 0.00
Phonons 0.02 0.06
SPUTTERING YIELD
Atoms/Ion
eV/Atom
TOTAL
Cr 0.000000 0.00
Fe 0.000000 0.00
Ni 0.000000 0.00
Save every 10000 ions
Random Number Counter 768944
HELP

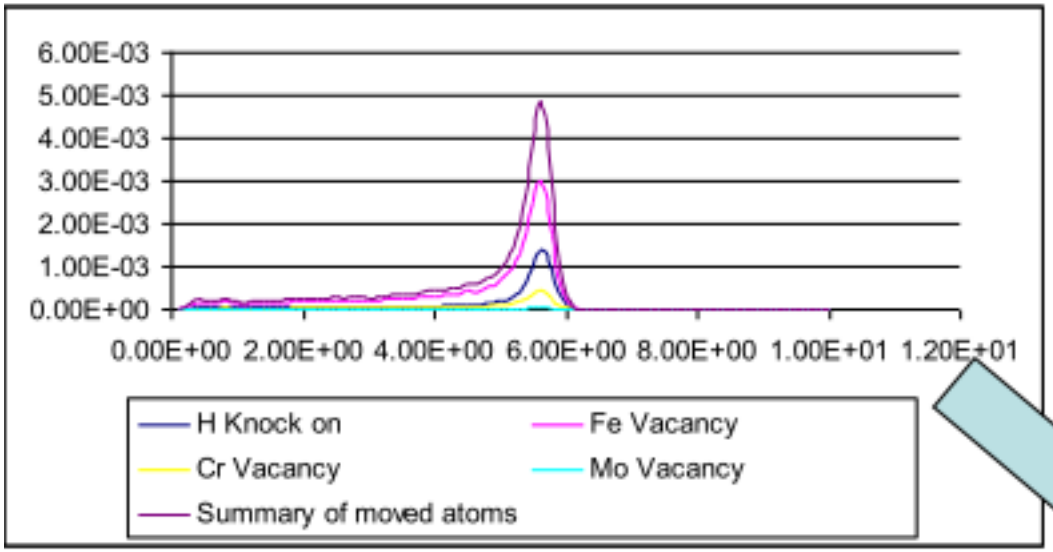
# Multilayer structures



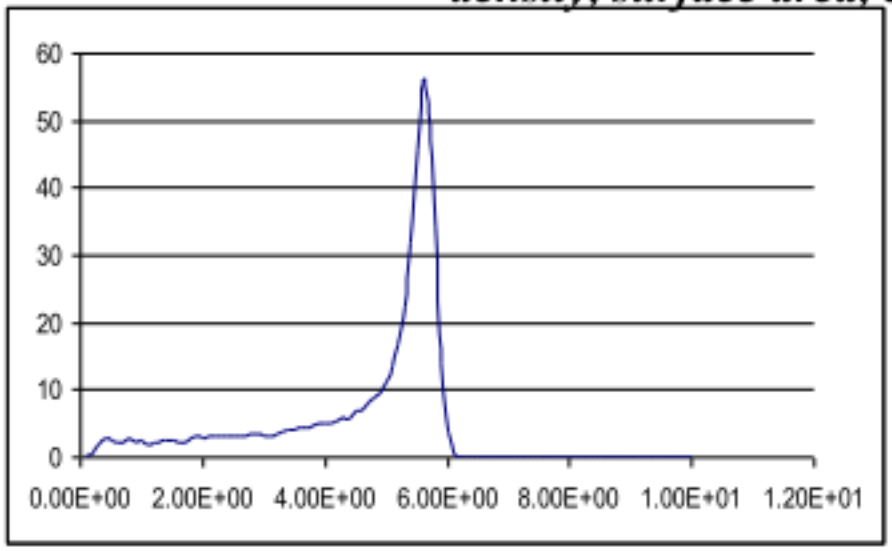

***SRIM is a very powerful and easy to use tool.***
***Multi layer systems are possible as well as angled impacts.***

# Dpa calc. using SRIM




***Vacancies produced in the material by incoming ion calculated using SRIM.***

***dpa in the material caused by the incoming ion with a given beam current, beam density, surface area, etc.***



# Vacancy output

```
====== H (3500) into Ta                                  =======
        SRIM-2003.26
=========================================
    Ion and Target VACANCY production
  See SRIM Outputs\TDATA.txt for calc. details
=========================================
====== TRIM Calc.=  H(3.5 MeV) ==> Ta(  50 um) ================================
-------------------------------------------------------------------------------
 See file :  SRIM Outputs\TDATA.txt for calculation data
 Ion    =  H   Energy = 3500 keV
============= TARGET MATERIAL ==========================================
Layer  1 : Ta
Layer Width =     5.E+05 A :
 Layer # 1- Density = 5.524E22 atoms/cm3 = 16.60 g/cm3
  Layer # 1- Ta = 100  Atomic Percent = 100  Mass Percent
===============================================================================
 Total Ions calculated =6984.00
 Total Target Vacancies     = 75 /Ion
 Total Target Displacements = 83 /Ion
 Total Target Replacement Collisions = 7 /Ion

!!!! NOTE : 2nd Column below is number of Primary Knock-Ons !!!!
          ( PKO are number of Target Atoms Recoiling from the Ion. )
=======================================================
  Table Units are  >>>> Vacancies / Angstrom / Ion  <<<<
=======================================================
   TARGET
   DEPTH          H           Ta
   (Ang.)     Knock-Ons    Vacancies
-----------  -----------  -----------
500001.E-02  3665.52E-09  1431.84E-08
100000.E-01  1323.02E-08  8287.51E-08
150000.E-01  1131.16E-08  6847.08E-08
200000.E-01  1239.98E-08  7903.78E-08
250000.E-01  1199.89E-08  7468.50E-08
```

***Sum of all ions***

# SRIM *dpa calc.*

***SRIM result=*** $\frac{\text{vacancies}}{\text{ion - Angstrom}}$

***dpa=Vac/(ion Å) * number of ions / number density***

***Number of ions:***

***Beam current I = A = C/sec***

***1e=1.6*10$^{-19}$ C***

} ***I * t / (1.6*10$^{-19}$)=ions***

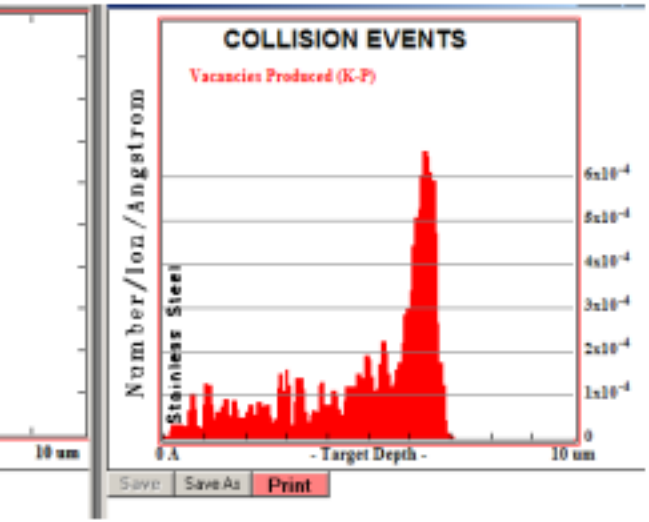
***Consider ion charge state!!***
***Consider irradiation area!!***

***Number density:***

***Atomic density *surface irradiated area=Atoms/cm$^3$*cm$^2$=Atoms/cm***

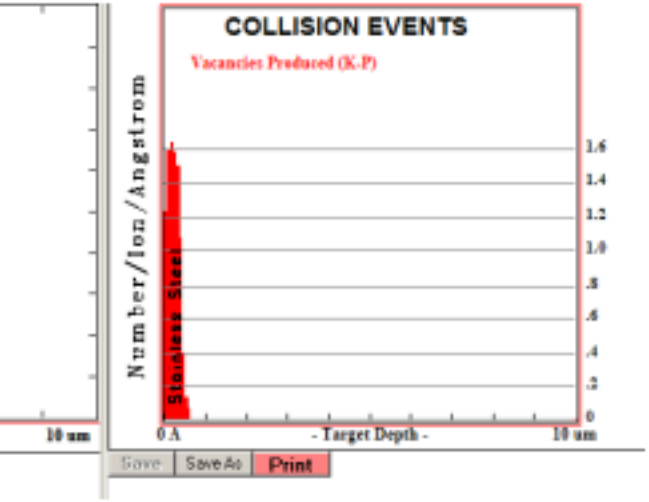
# *WATCH UNITS !!!!!!!!!!!!!!!!!!!!!*

# Ion comparison with SRIM



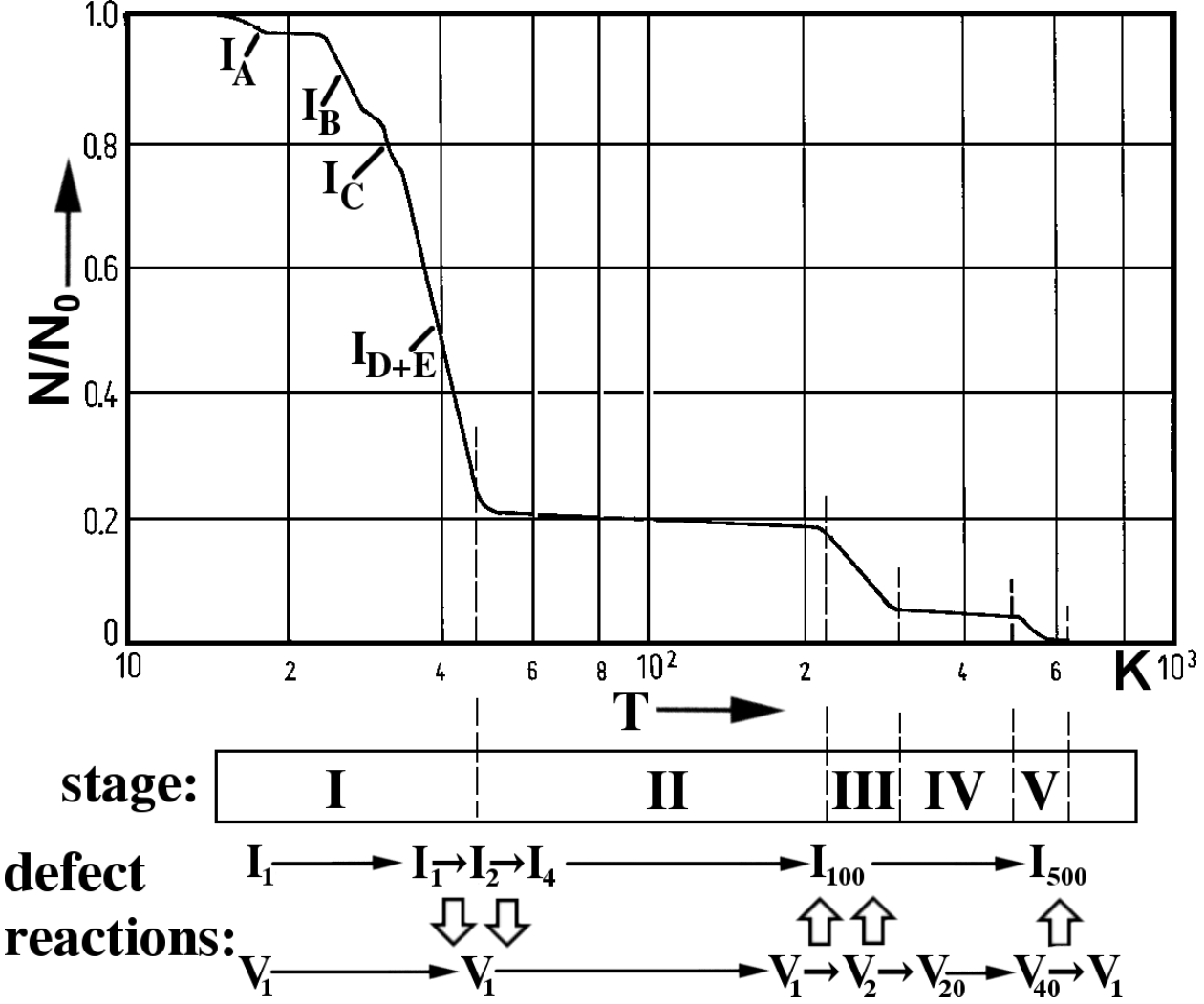

*1MeV protons in stainless steel*

***Heavier ions cause more damage!***
***Lighter ions are going deeper into the material than heavier ions***
***Heavier ions cause higher dose rate.***




*1MeV $Fe^{2+}$ in stainless steel*

So we created displacements.
So What??




Five recovery stages in electron-irradiated Cu *I* and *V* denote single interstitials and vacancies, respectively; and *I*2 and *V*2, di-interstitials.

**Stage I:** The lower temperature substages *IA*, *IB*, and *IC* are due to collapse of close Frenkel pairs. *ID* is due to correlated recombination and *IE* due to uncorrelated recombination.

**Stage II:** Interstitial clusters grow, leading to identifiable small interstitial loops.

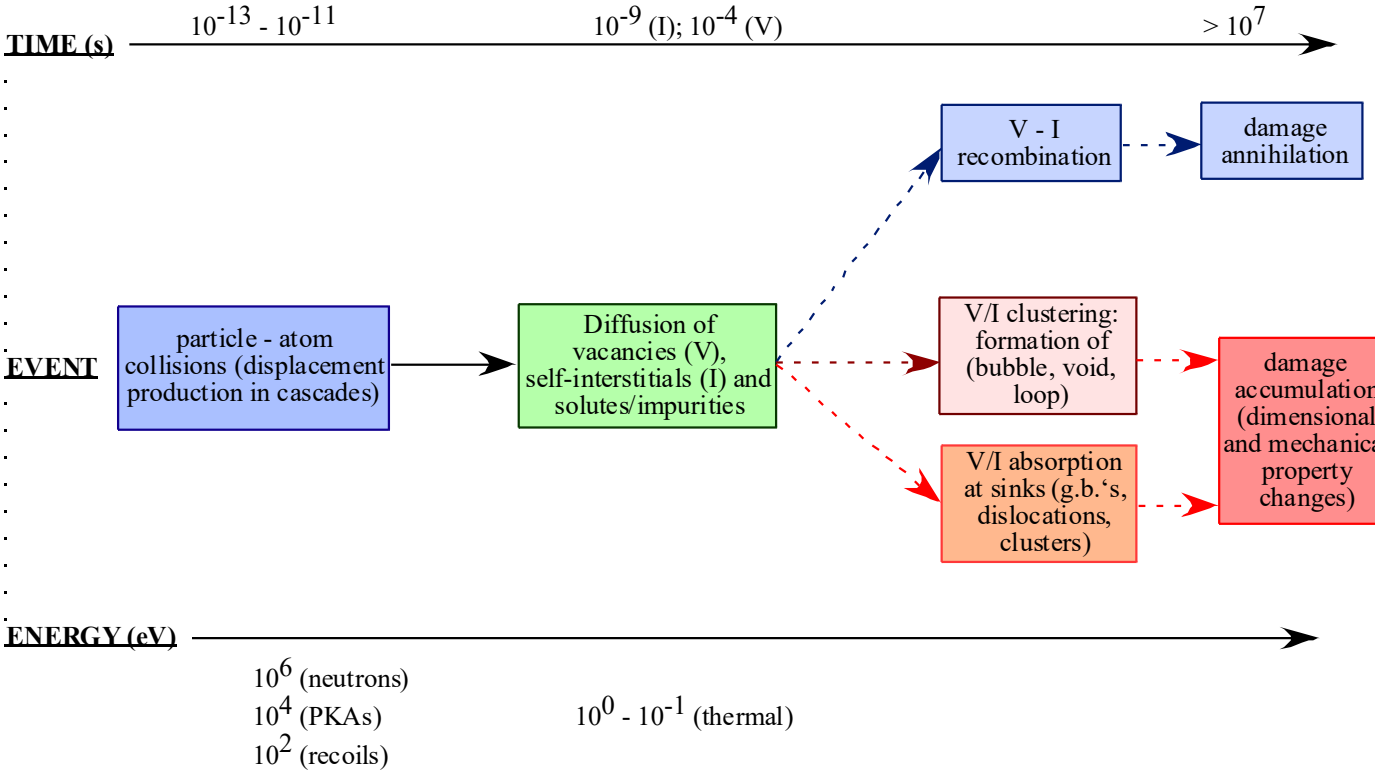
**Stage III:** Vacancies migrate and adulate at interstitial clusters.

**Stage IV:** The vacancy clusters surviving stage III grow in size. The vacancy clusters dissociate thermally.

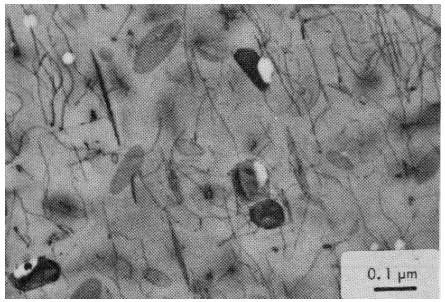
# *Fate of the displaced atoms*

- Recombination of vacancies and interstitials: **V + I → null** (perfect lattice)
- **Vacancies** coalesce into:
  - small clusters (depleted zones or *displacement spikes*) - in fcc metals, these are usually stacking fault tetrahedra (SFT); in bcc metals, these are ultra-small, sub-nanometer cavities (nanovoids)
  - large clusters (voids or cavities)
- **Interstitials** coalesce into dislocation loops
- It is these point defect clusters (along with radiation induced/enhanced diffusion, precipitation and segregation) that are responsible for mechanical (hardening and embrittlement) and/or physical property changes

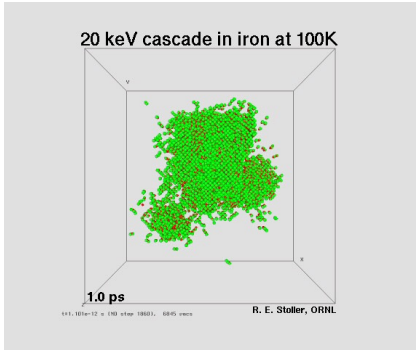
# Radiation effects are governed by the ultimate fate of point defects (& transmutants)



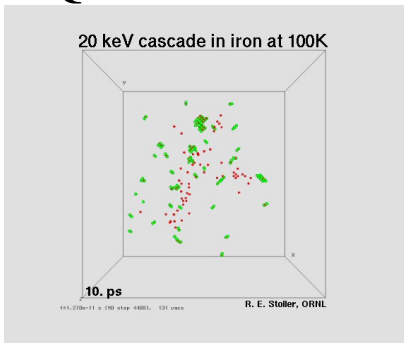

Voids, I-loops & precipitates in stainless steel




**Nascent cascade**




**"Quenched" cascade**

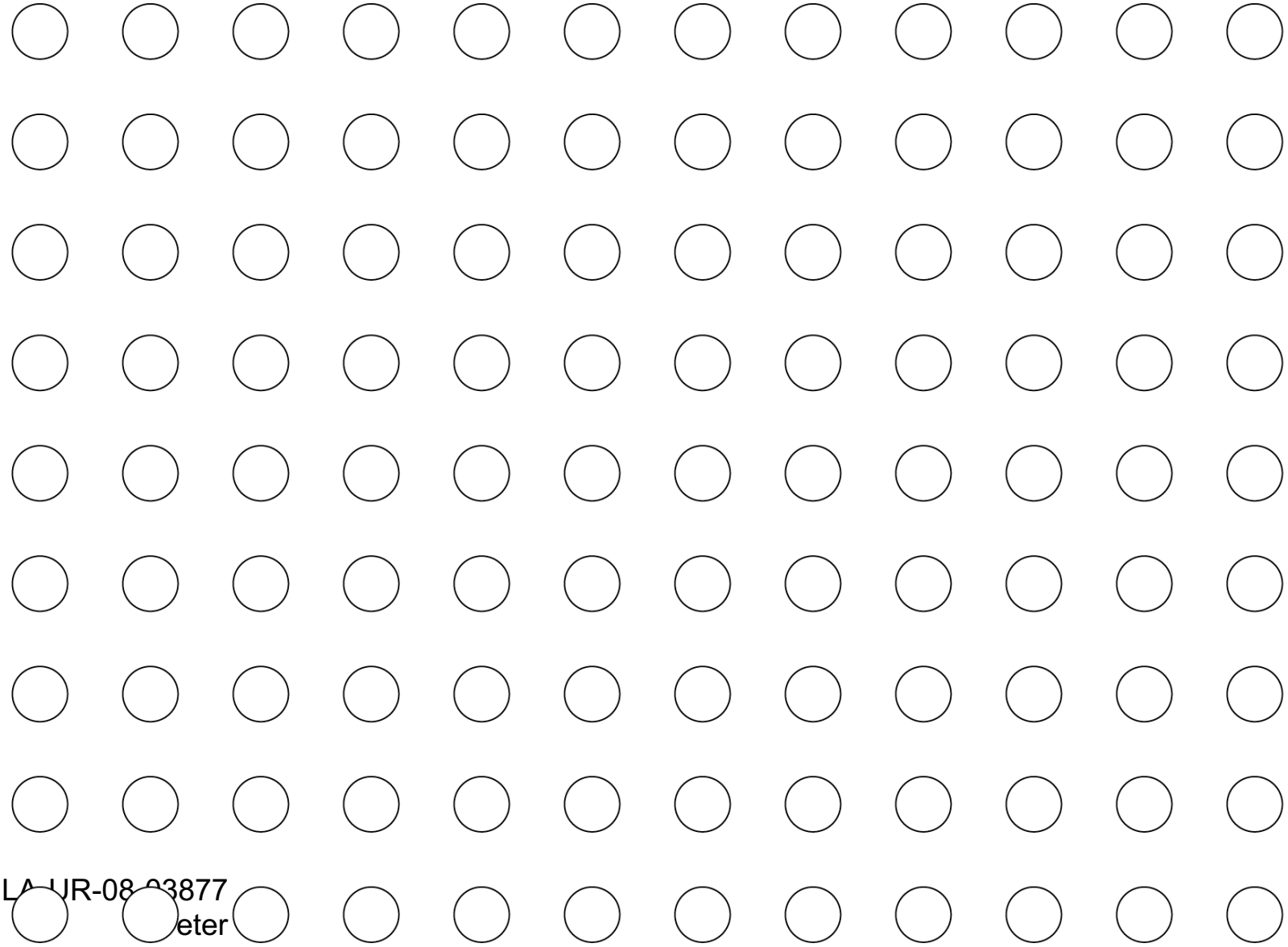



**Number of defects:**

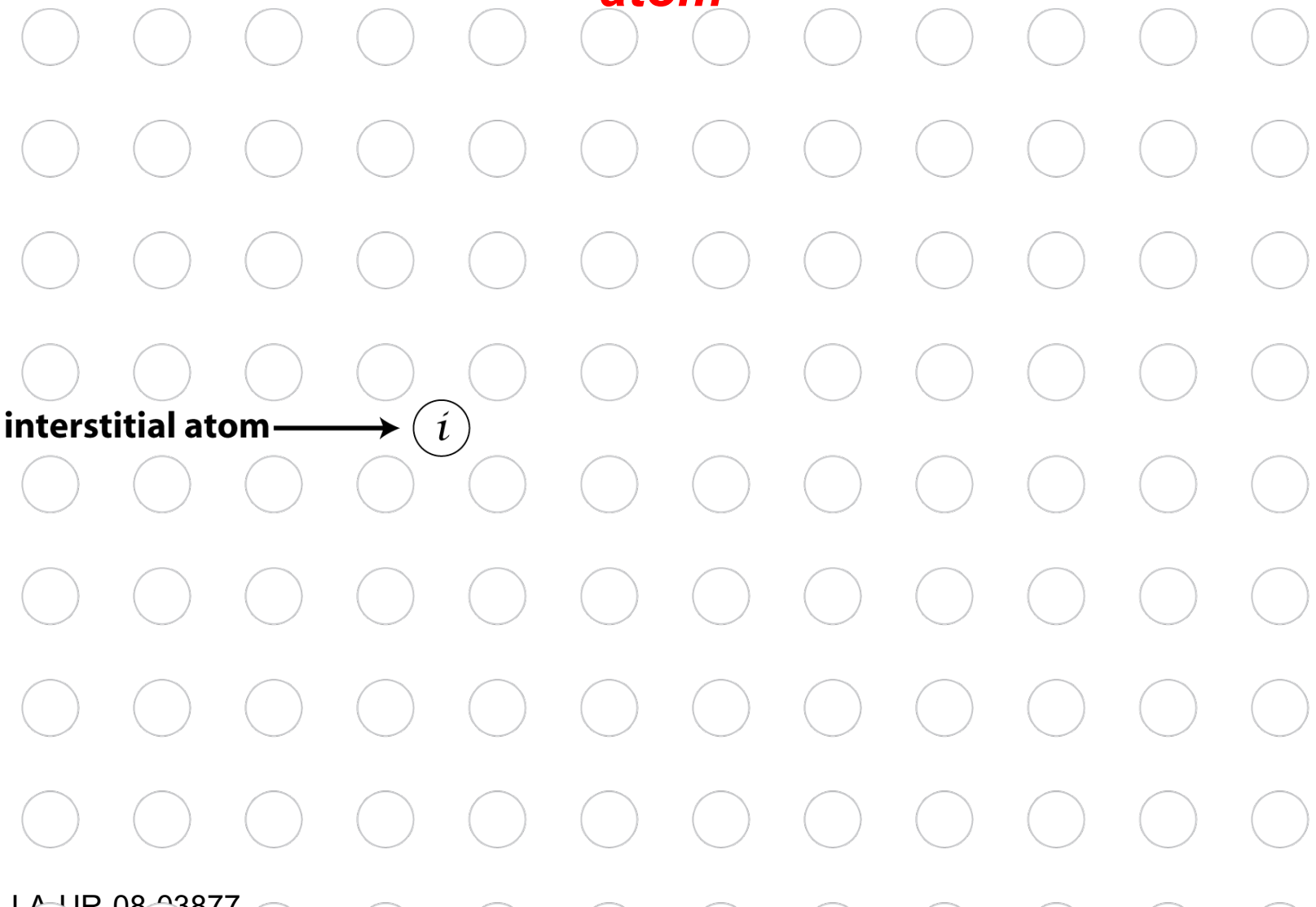
**Nascent cascade: $N_i = N_v = \nu(T)$**

**"Quenched" cascade: $N_i' = N_v' < \nu(T)$**

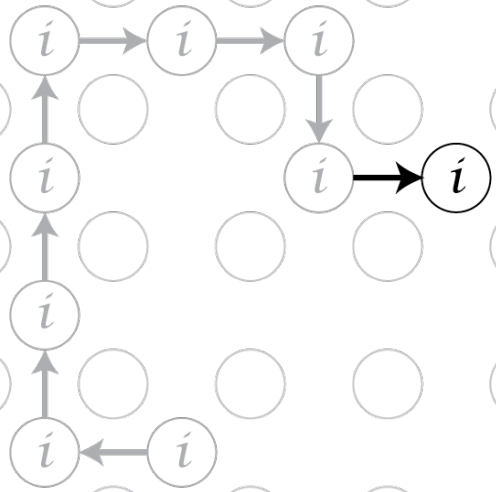
# Formation of dislocation loops in a perfect lattic



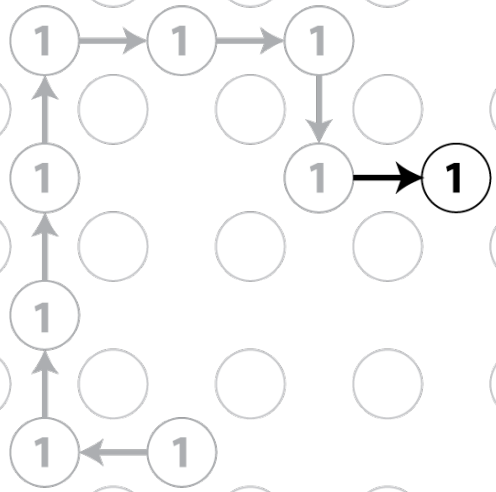
# *Perfect Lattice + Interstitial Point Defect*
# *In a monoatomic solid, this would be called a self-interstitial atom*



# Perfect Lattice + Freely-Migrating Self-Interstitial Atom (SIA)

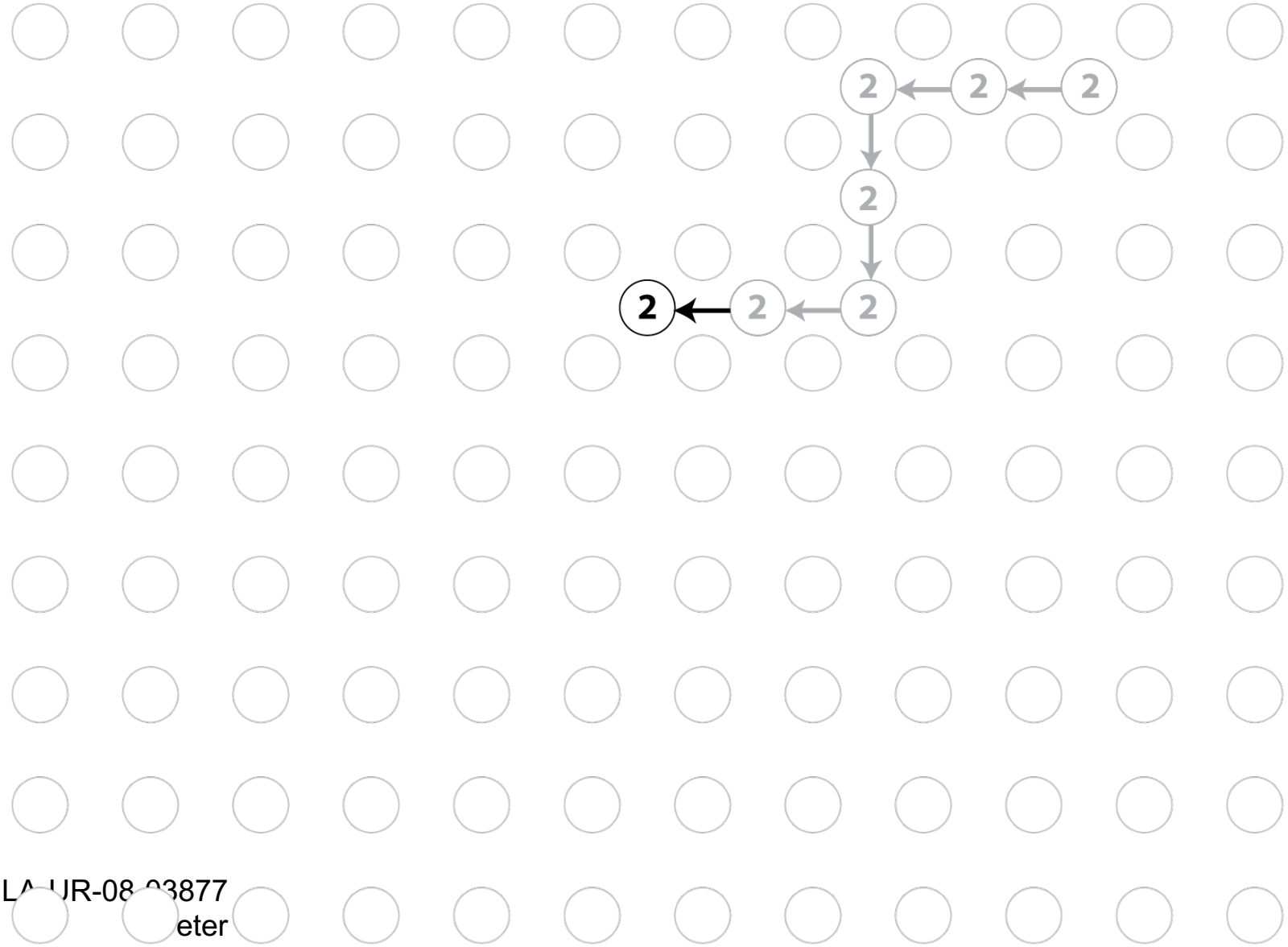


# Perfect Lattice + Freely-Migrating SIA #1




LA-UR-08-03877
Peter
Hosemann

# Perfect Lattice + Freely-Migrating SIA #2

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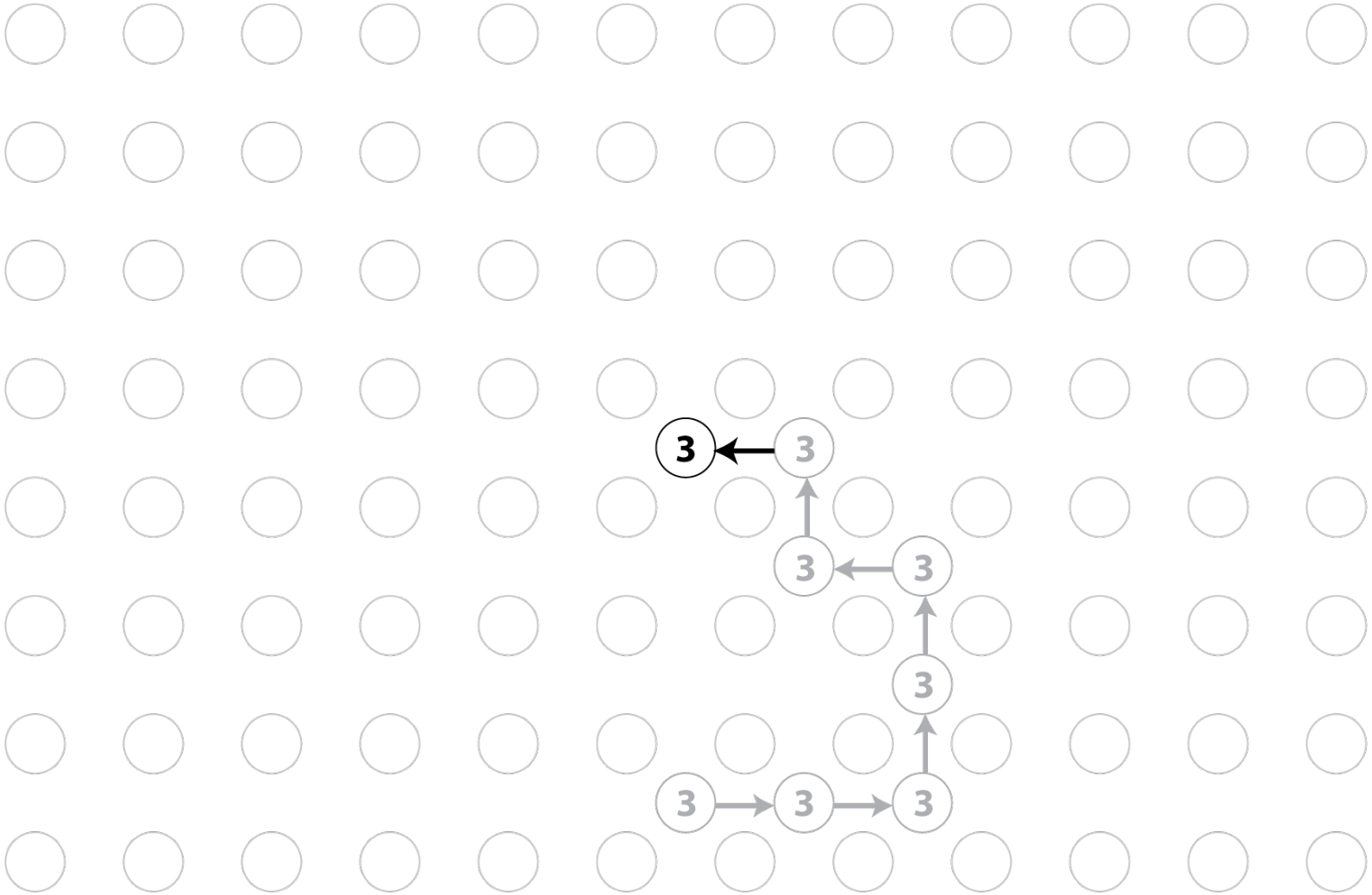
# Perfect Lattice + Freely-Migrating SIA #3

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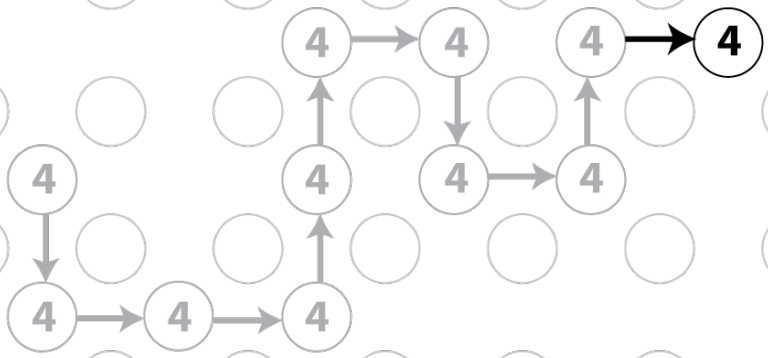
# *Perfect Lattice + Freely-Migrating SIA #4*

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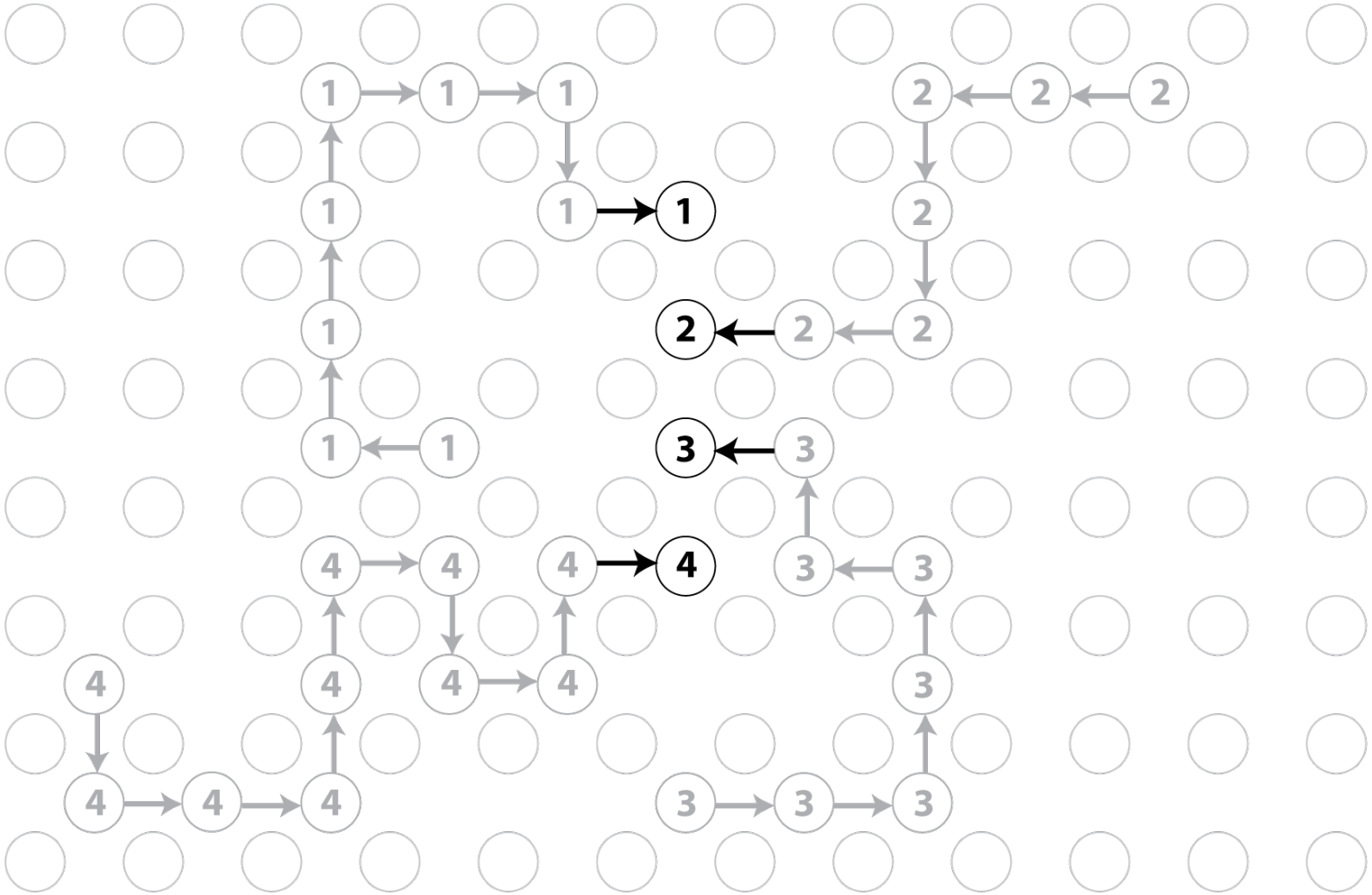
# *Perfect Lattice + Several Freely-Migrating SIAs*



# *Perfect Lattice + Interstitial Loop*
# *Loop condensed from freely-migrating SIAs*

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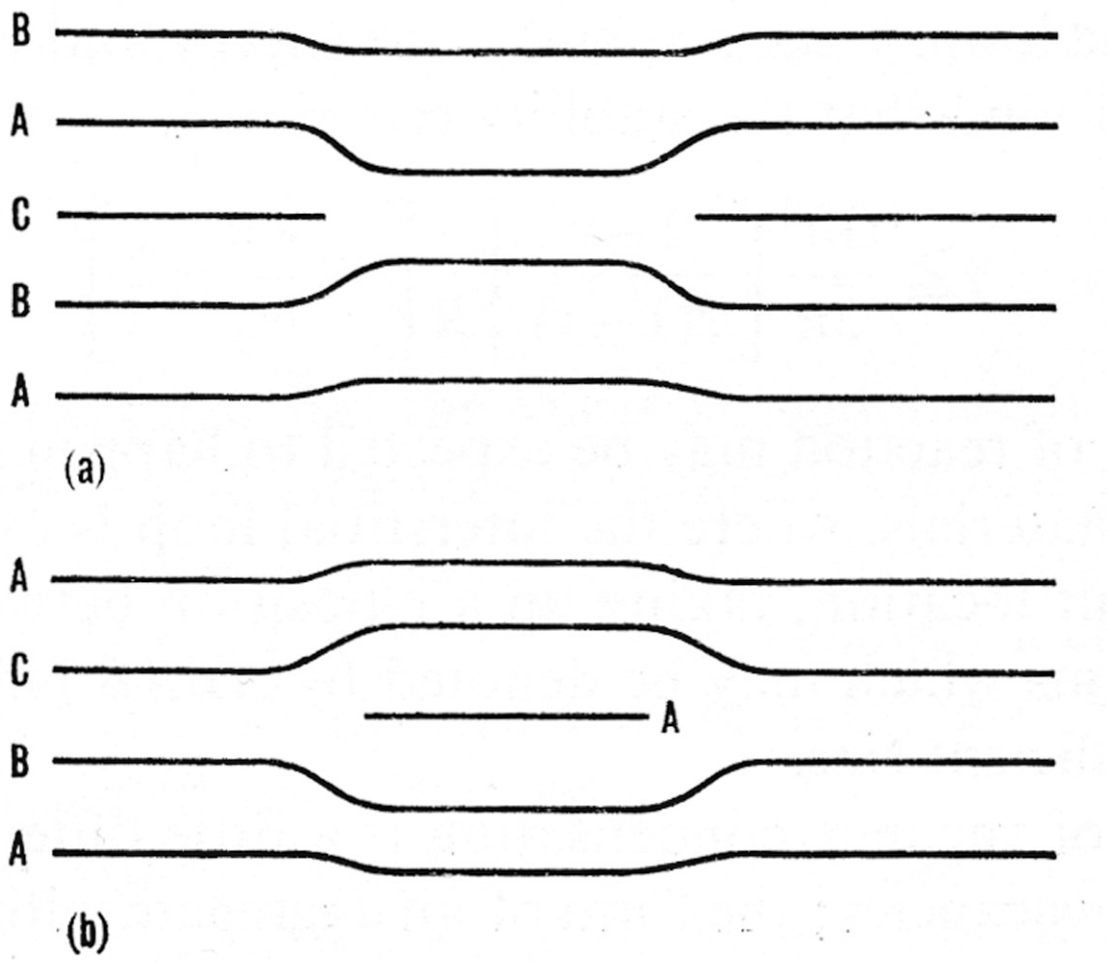
# Dislocation loops

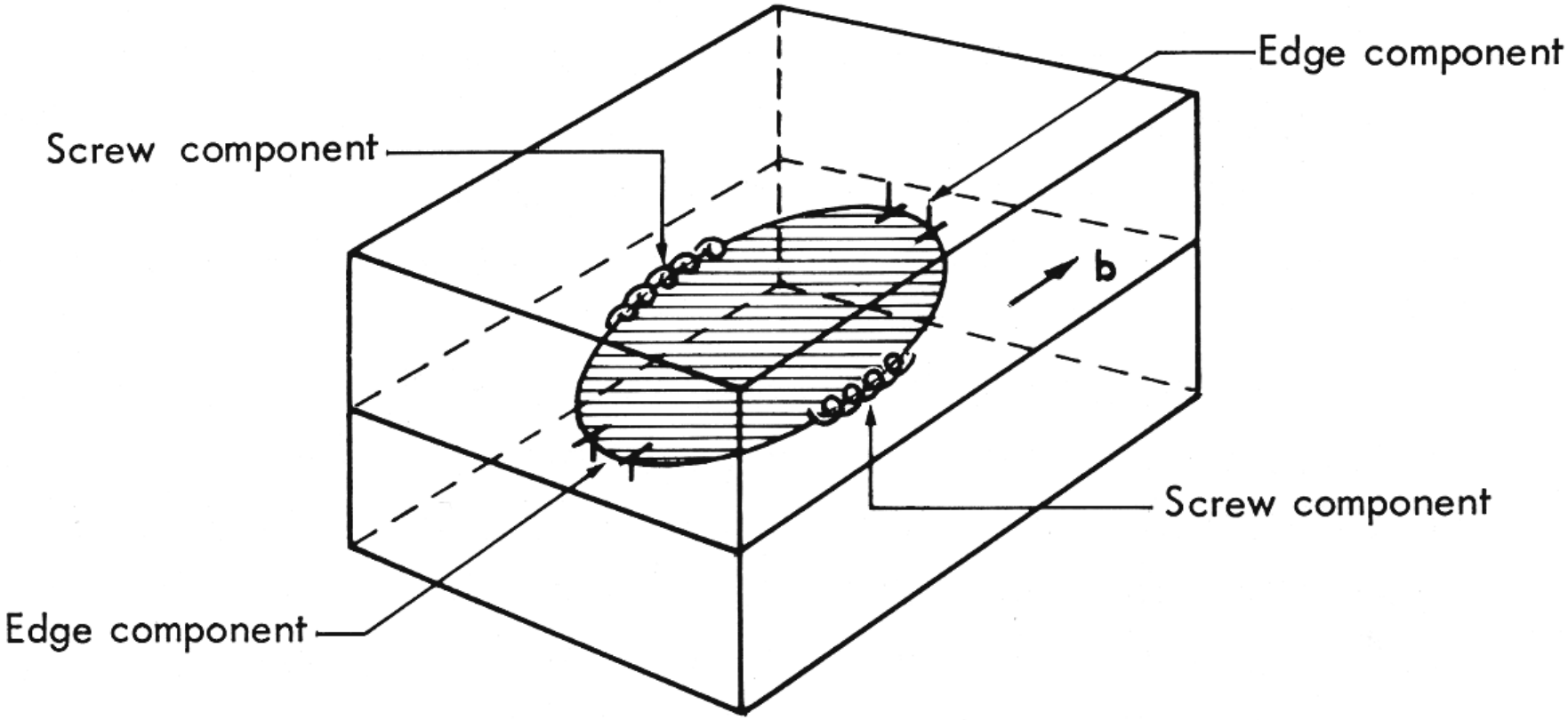



***(a) Condensation of vacancies to form a vacancy loop (a missing plane of atoms)***

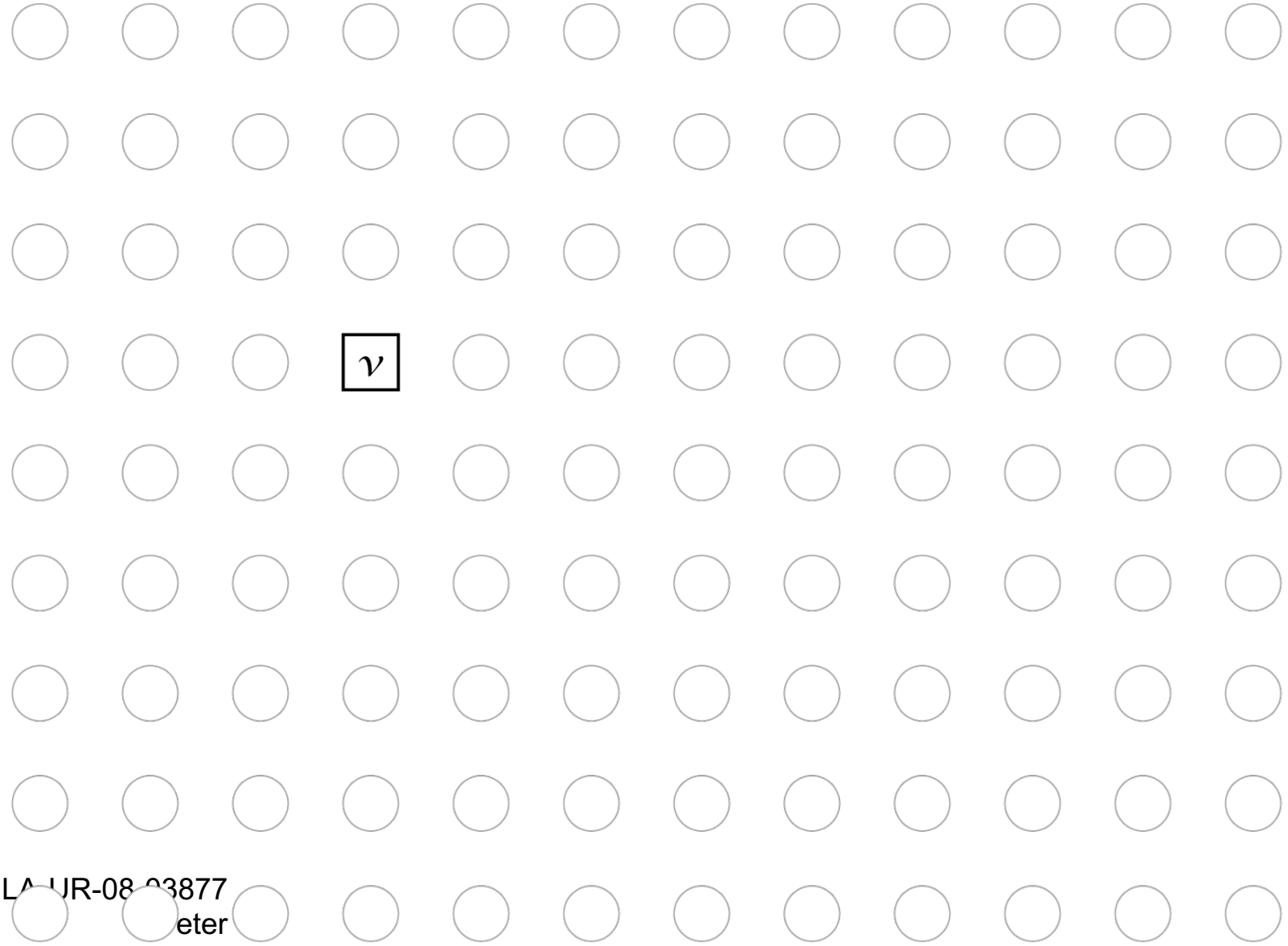
***(b) Condensation of interstitials to form an interstitial loop (an extra plane of atoms)***

# Dislocation Loops II

***Top-View of Loop***



# *Void formation:*
# *Perfect Lattice + Vacancy Point Defect*

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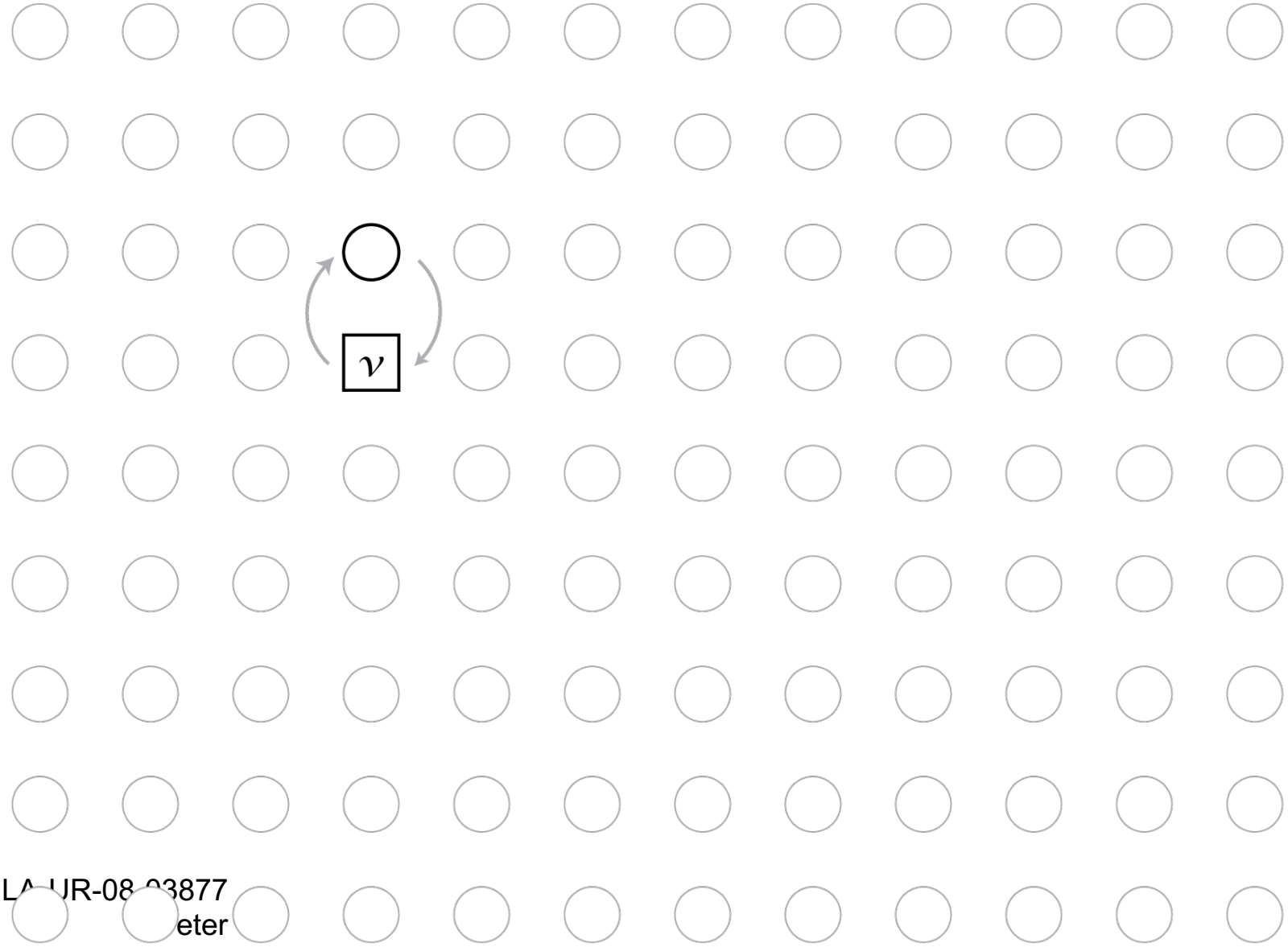
# Vacancy Before Migration

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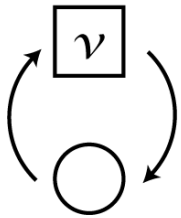
# Vacancy After Migration

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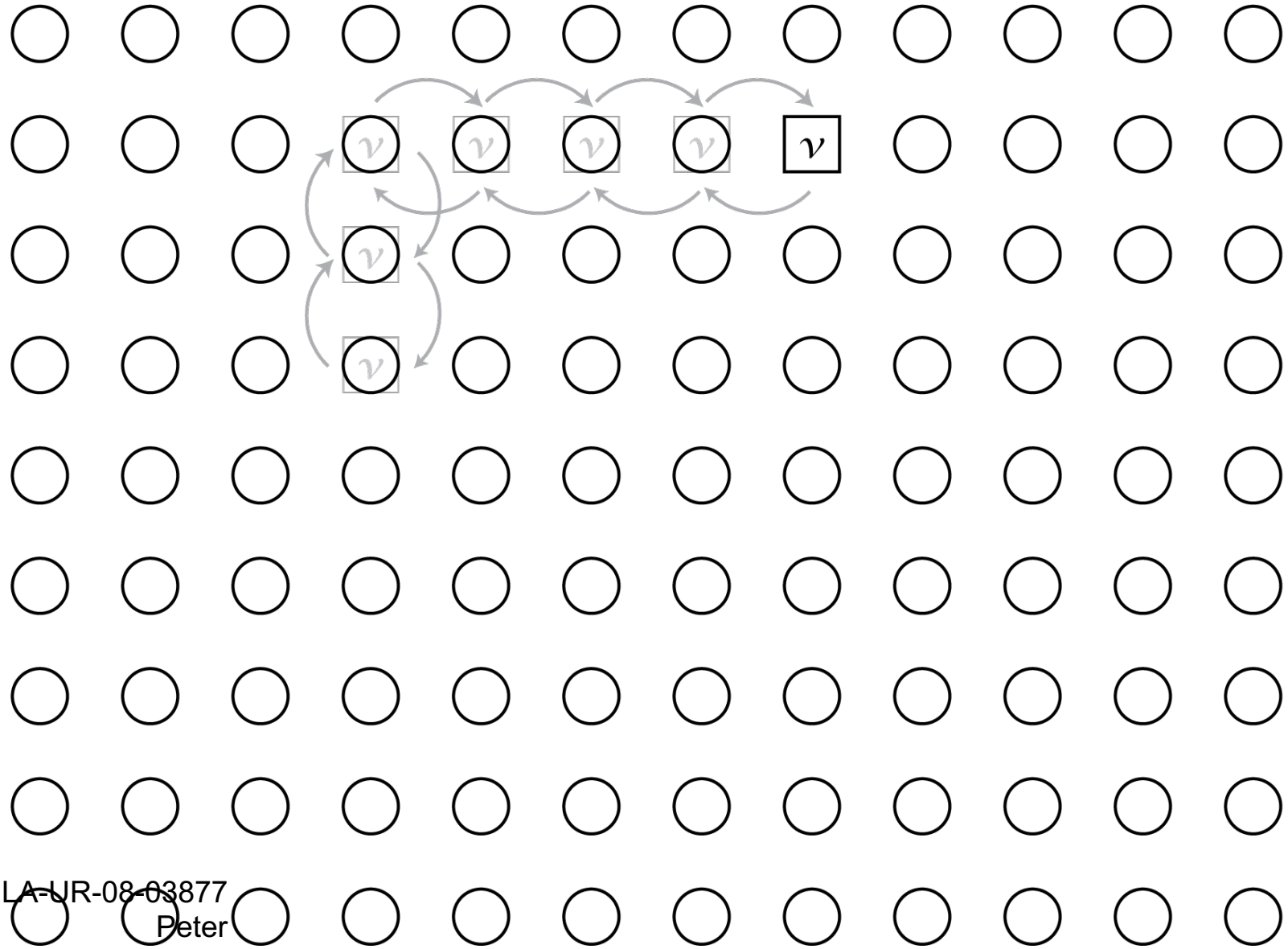
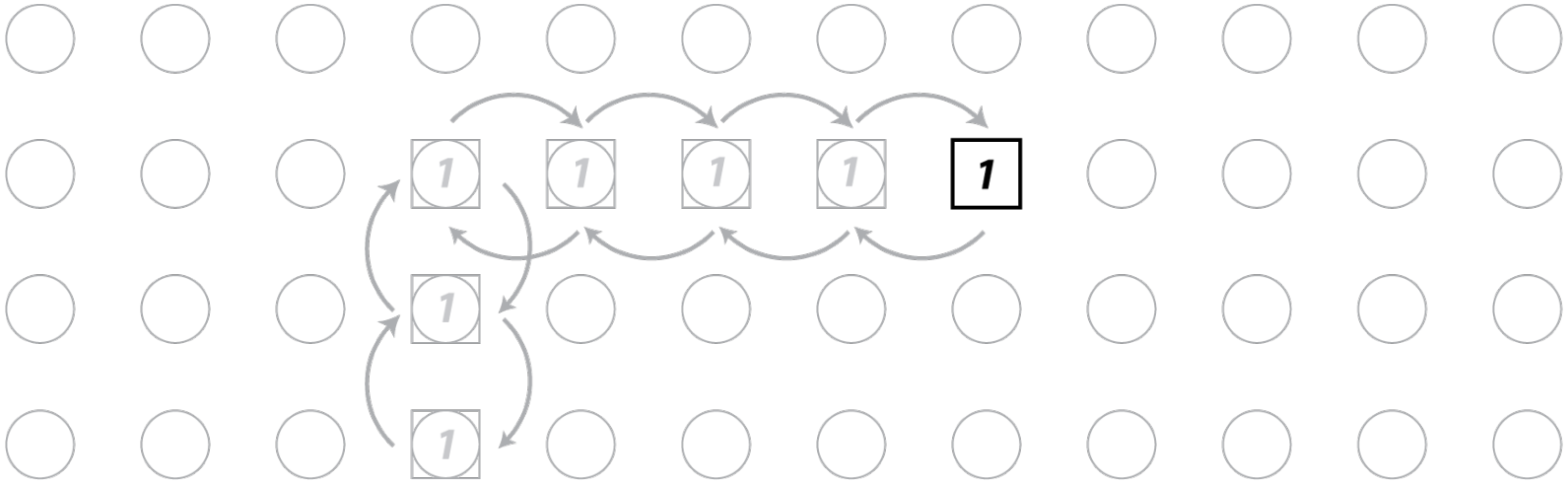
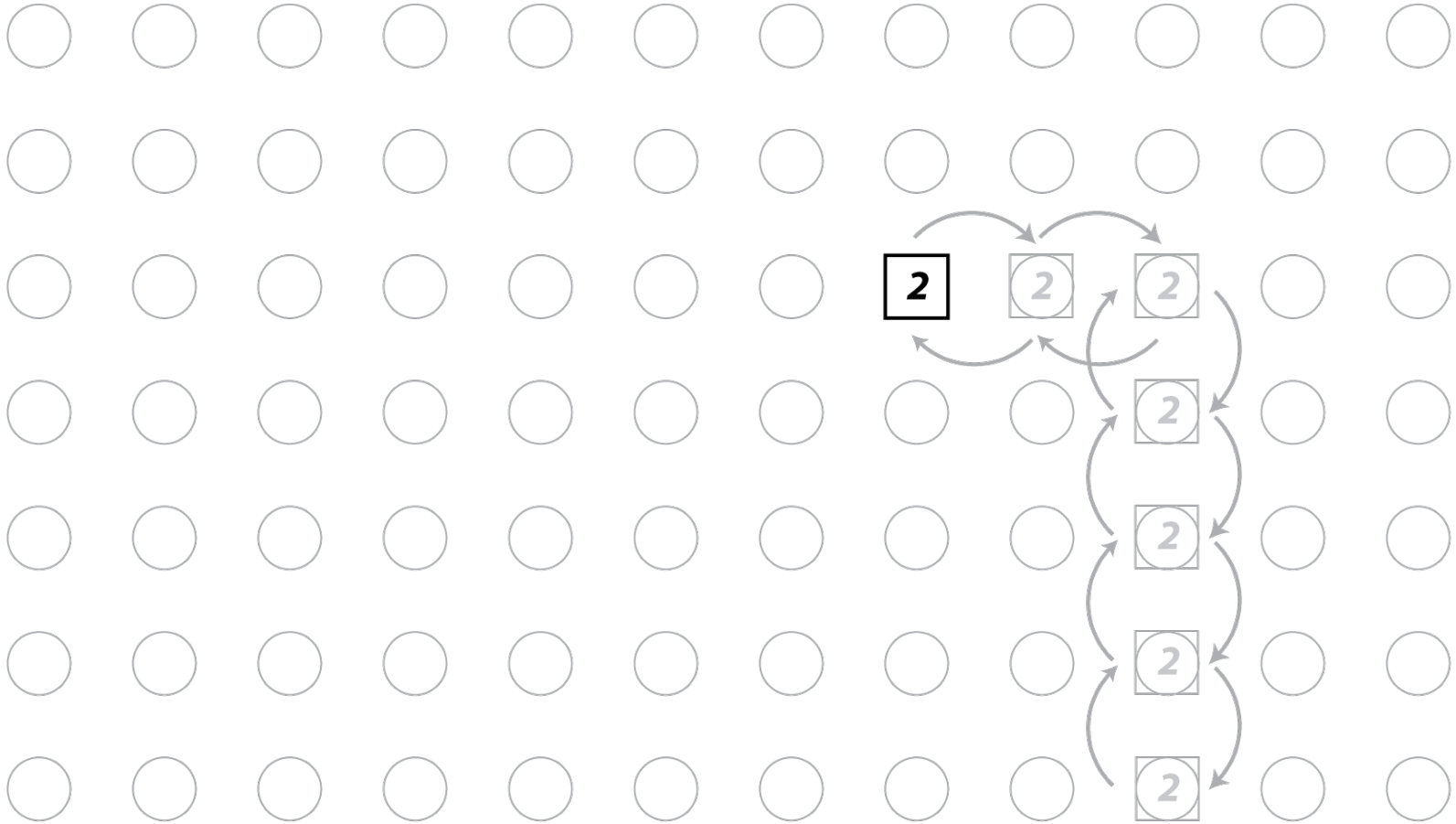
# Perfect Lattice + Freely-Migrating Vacancy



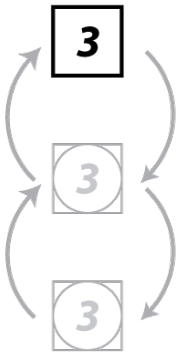
# *Perfect Lattice + Freely-Migrating Vacancy #1*



# Perfect Lattice + Freely-Migrating Vacancy #2



# *Perfect Lattice + Freely-Migrating Vacancy #3*

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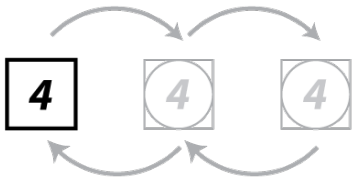
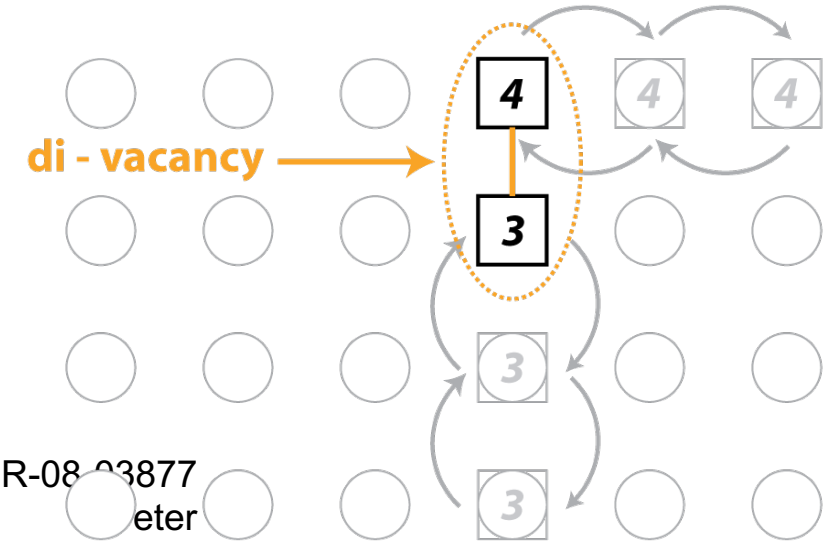
# Perfect Lattice + Freely-Migrating Vacancy #4



# Di - Vacancy Formation

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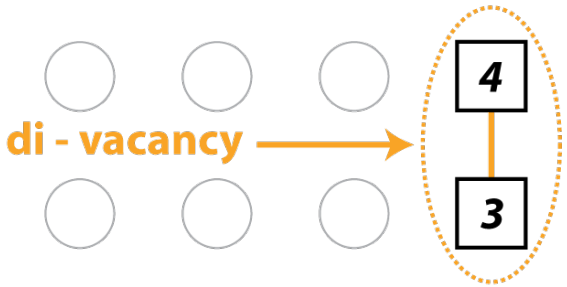
# Di - Vacancy Formation

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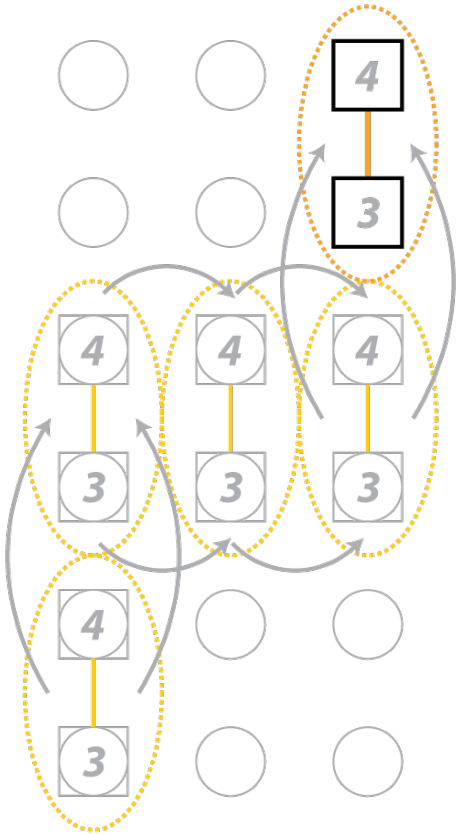
# Di - Vacancy Migration

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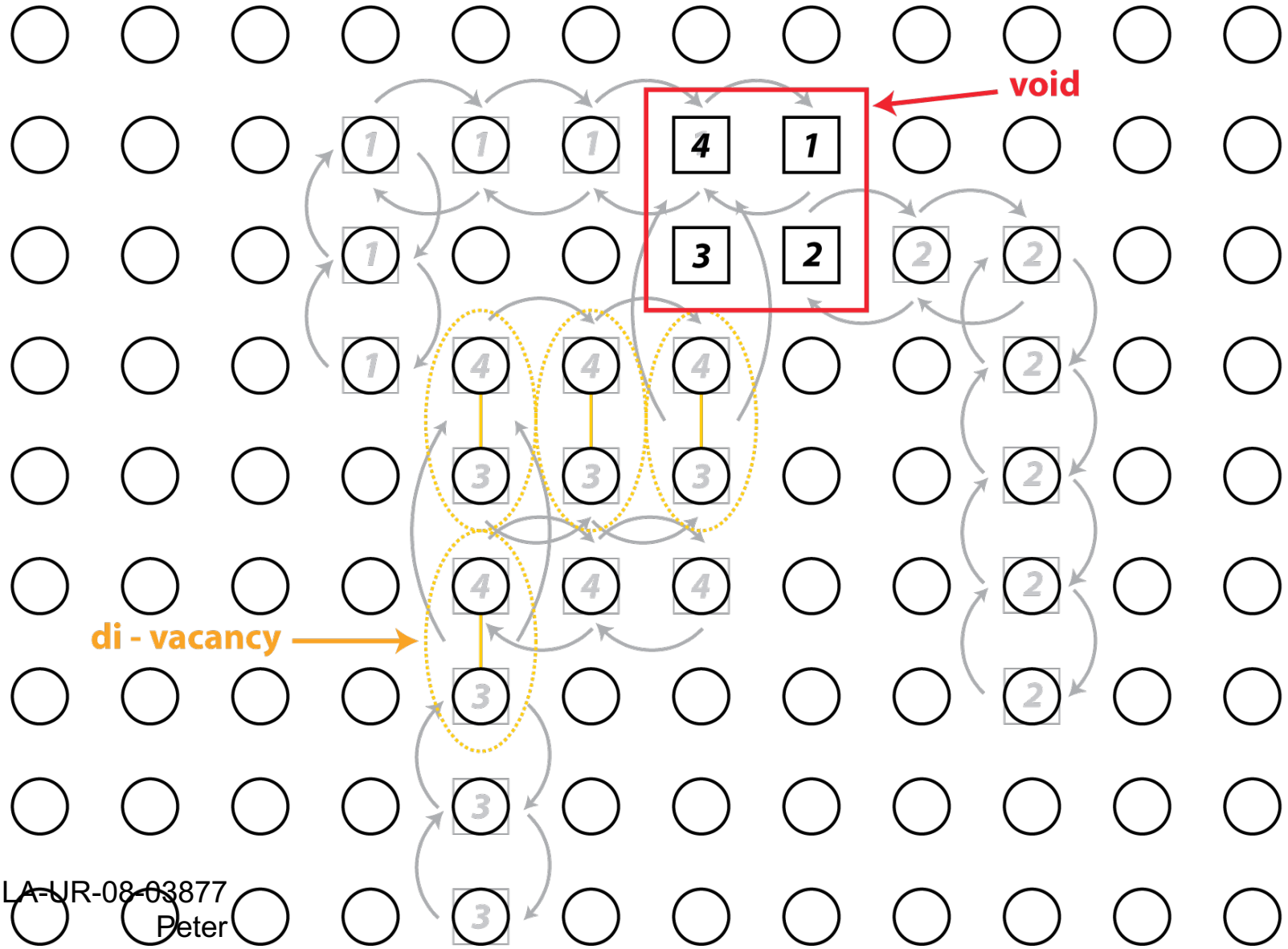
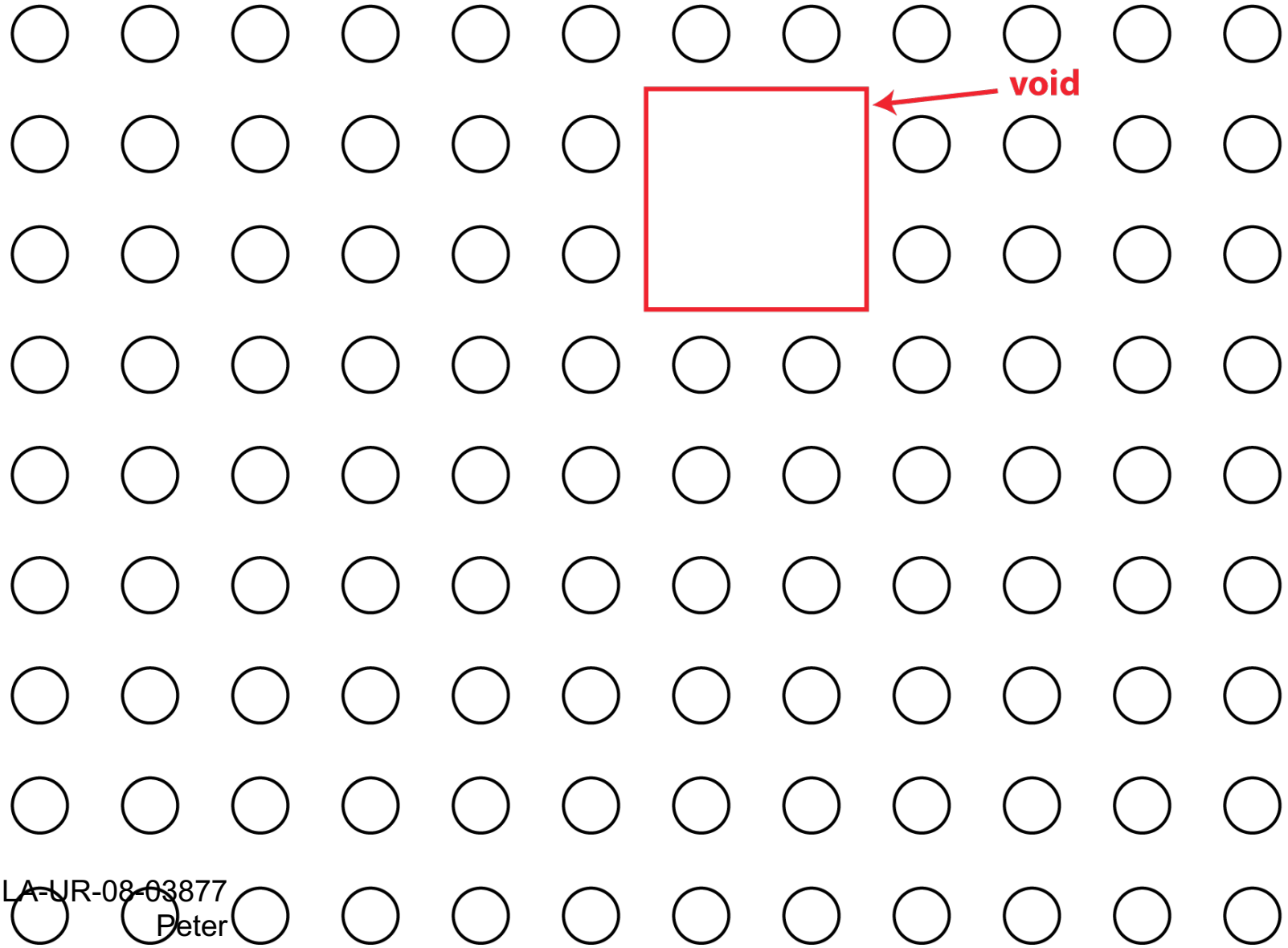
# Freely-Migrating Vacancy Point Defects - Void Nucleation



# Freely-Migrating Vacancy Point Defects - Void Formation

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# Void swelling effects