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ADVANCED MATERIALS RESEARCH & INNOVATION

ROYCE

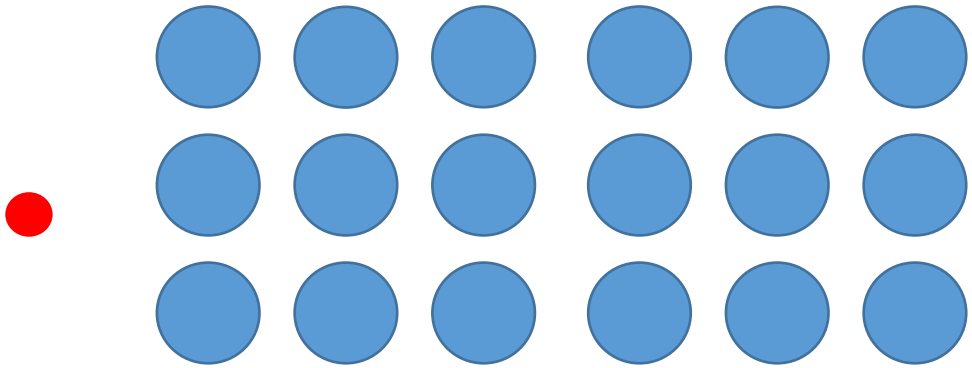
# Best practice for SRIM radiation damage calculations

Dr Robert Harrison

The University of Manchester is the Hub of the Henry Royce Institute for advanced materials

# Displacement theory

- Neutron strikes atom in material and displaces it giving it energy *T*
- Known as the Primary Knock on Atom (PKA) – if energy high enough causes other displacements (Secondary Knock on Atoms and so on)
- Causes the formation of many defects (interstitials and vacancies) in the material
- Need to develop a model to calculate the number of atoms displaced by the PKA

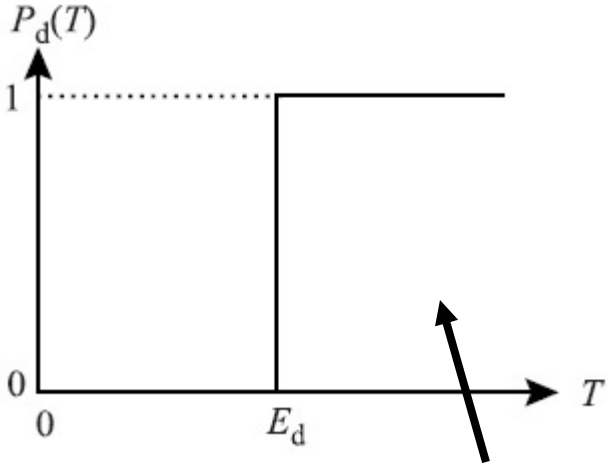


# Probability of displacement

- The probability of a **displacement ($P_d$)** of an atom struck with energy *T* has a minimum energy

$P_d(T) = 0$ when $T < E_d$

$P_d(T) = 1$ when $T > E_d$




- <u>However, it is not that simple!</u>

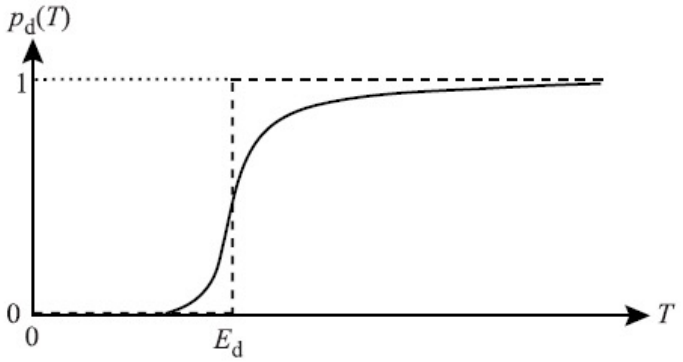
- There is no single value for $E_d$ for all collisions due to;
  - Crystallographic effects
  - Direction of PKA (random but effects recoil)
  - The thermal energy in the lattice atom

**This is only true for an amorphous material at 0 K**

$P_d(T) = 0$ when $T < E_{dmin}$

$= 0\text{-}1$ when $E_{dmin} < T < E_{dmax}$

$= 1$ when $T > E_{dmax}$




Was G.S. (2017) The Displacement of Atoms. In: Fundamentals of Radiation Materials Science. Springer, New York, NY.

# Displacement energy ($E_d$)

- The table shows some typical metals used in the nuclear industry along with their minimum and average displacement energies ($E_d$)
- The single average $E_d$ is used in DPA calculations – calculated form the average of the crystallographic specific values

| Metal | $E_{dmin}$ /eV | $E_d$/eV |
|---|---|---|
| Al | 16 | 25 |
| Ti | 19 | 30 |
| Cu | 19 | 30 |
| Zr | 21 | 40 |
| W | 40 | 90 |
| Ta | 34 | 90 |
| Fe | 20 | 40 |
| Stainless steel | | 40 |

# The Kinchin and Pease (KP) model

- In 1955 Kinchin and Pease developed a simple model for calculating the number of displaced atoms based on the following assumptions;

1) All collisions are two-body elastic collisions (i.e. one collision at a time)

2) The displacement probability ($P_d(T)$) = 1 for $T > E_{d,}$ the arrangement of atoms is random (amorphous) – no crystallographic effects, no temperature effects

3) All energy is transferred between the PKA and recoil atom during the collision – i.e. there is no other energy loss to the lattice (making it vibrate)

4) Energy loss to the electronic system is given by a cut off $E_c$ – if the PKA has a higher energy than this, no more displacements are caused (see later on)

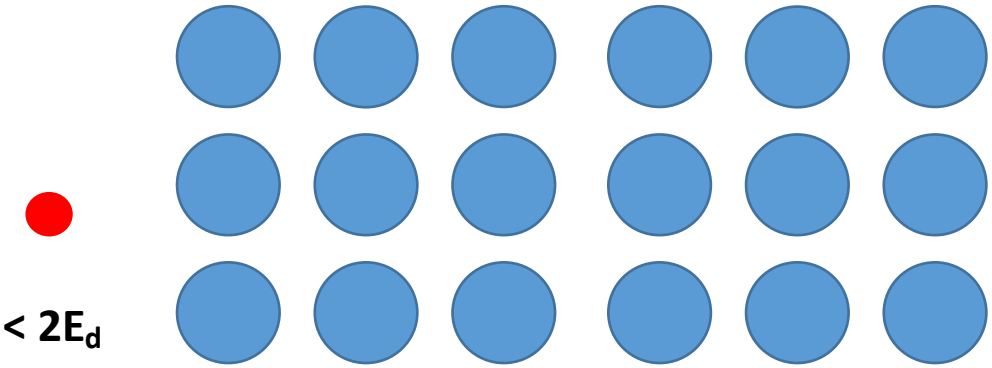
5) The energy transfer cross section is given by the hard-sphere model (i.e. atoms are hard spheres and they cannot overlap in space)

# The Kinchin and Pease (KP) model

- So the KP model states that;

$$v(T) = 0 \text{ when } T < E_d$$

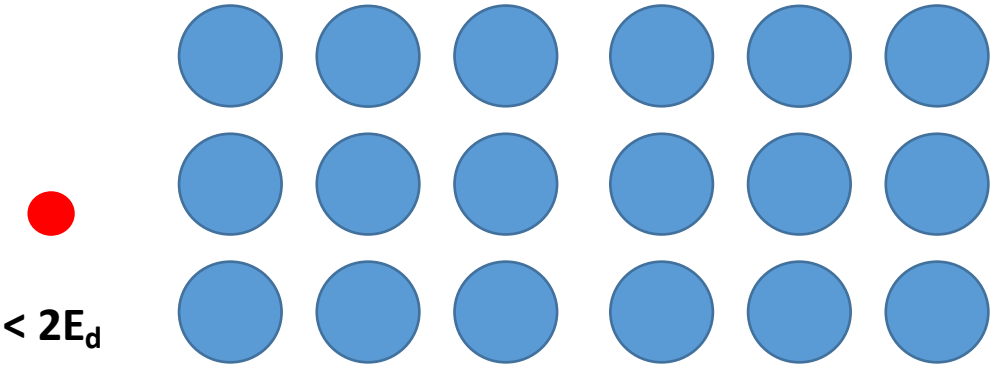
- What about when struck atom has energy $T$ greater than $E_d$ but less than $2E_d$?



$E_d < T < 2E_d$

The PKA does not transfer $E_d$

$$v(T) = 1$$



$E_d < T < 2E_d$

The PKA does transfer $E_d$

But is captured by the vacant site – **a replacement collision**

$$v(T) = 1$$

**(actually 2 displacements have happened!)**

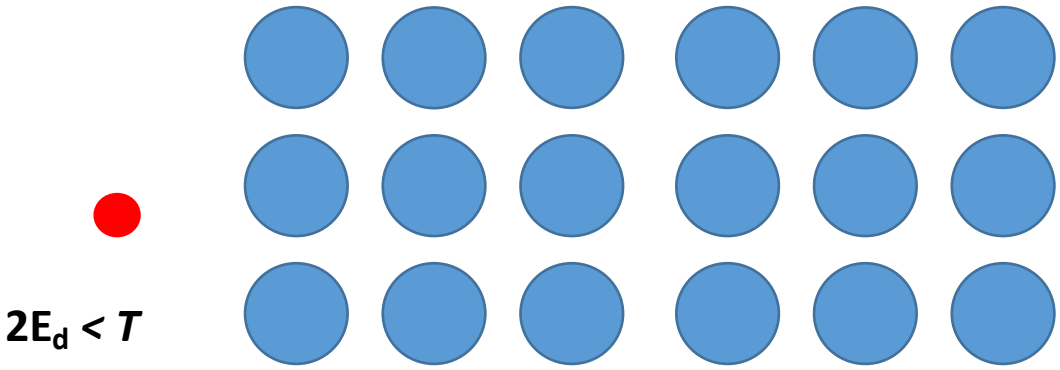
# The Kinchin and Pease (KP) model

- So now we can say the KP model states that;

$$v(T) = 0 \text{ when } T < E_d$$

$$v(T) = 1 \text{ when } E_d < T < 2E_d$$

- Now what about when struck atom has energy (*T)* greater than $2E_d$?



**$2E_d < T$**

The PKA can now transfer energy $E_d$ to a second atom but still has $T > E_d$

Enough energy to keep going, so;

$$v(T) > 1 \text{ when } 2E_d < T$$

$$v(T) = \frac{T}{2E_d}$$

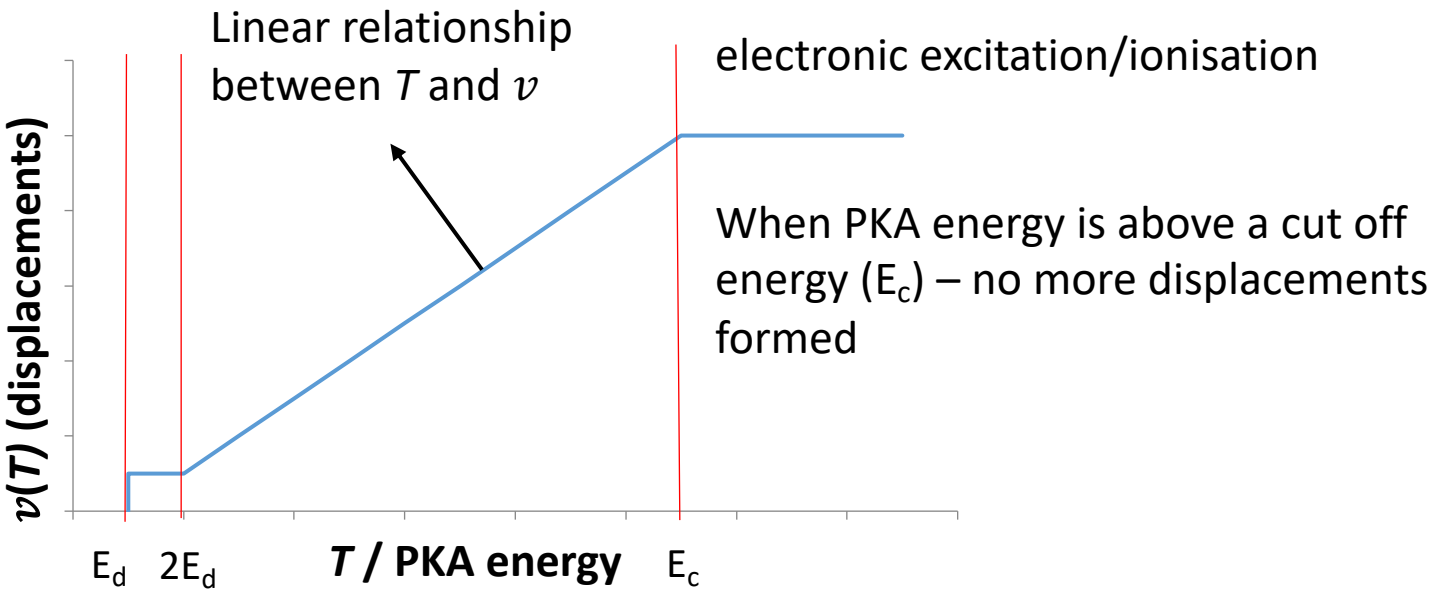
# The Kinchin and Pease (KP) model

- So now we can say the KP model states that;

$v(T) = 0$ when $T < E_d$

$v(T) = 1$ when $E_d < T < 2E_d$

$v(T) = \frac{T}{2E_d}$ when $2E_d < T < E_c$

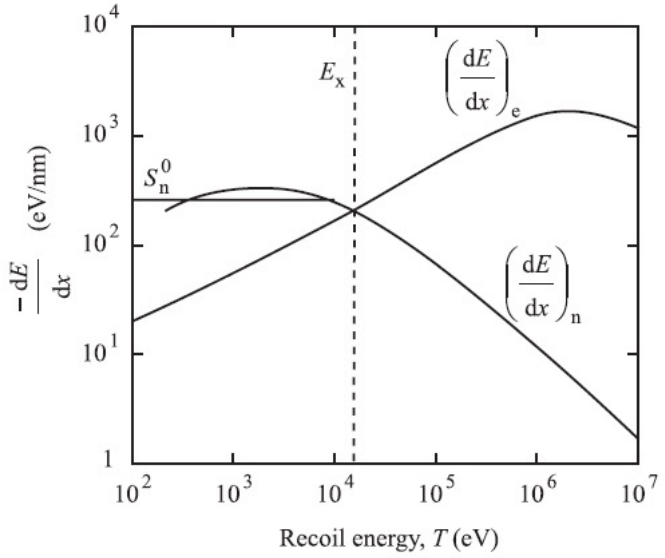


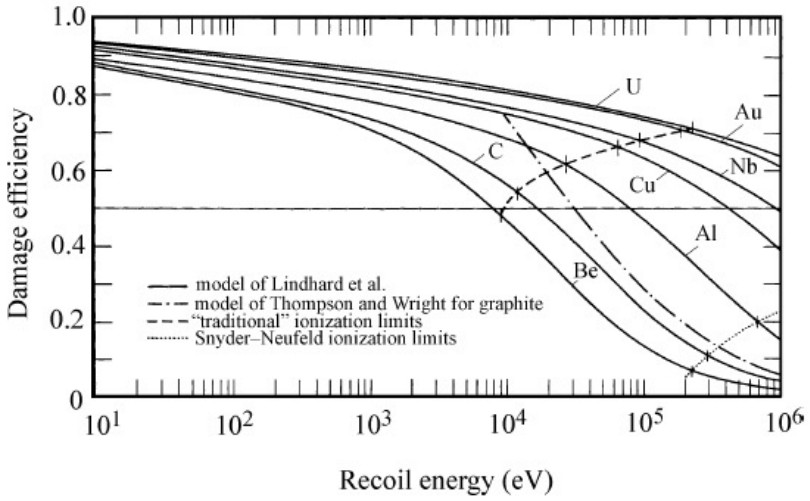
# The NRT modified KP model

- Modifications of the KP model were made by Norgett, Robinson and Torrens (NRT) in 1975 - Still used in todays calculation of radiation damage in nuclear materials!

- They modified some of the assumption made in the KP model, namely;

    4) **Energy loss to the electronic system is given by a cut of $E_c$ – if the PKA has a higher energy than this, no more displacements are caused**
    5) The energy transfer cross section is given by the hard-sphere model (i.e. atoms are hard spheres and they cannot overlap in space)

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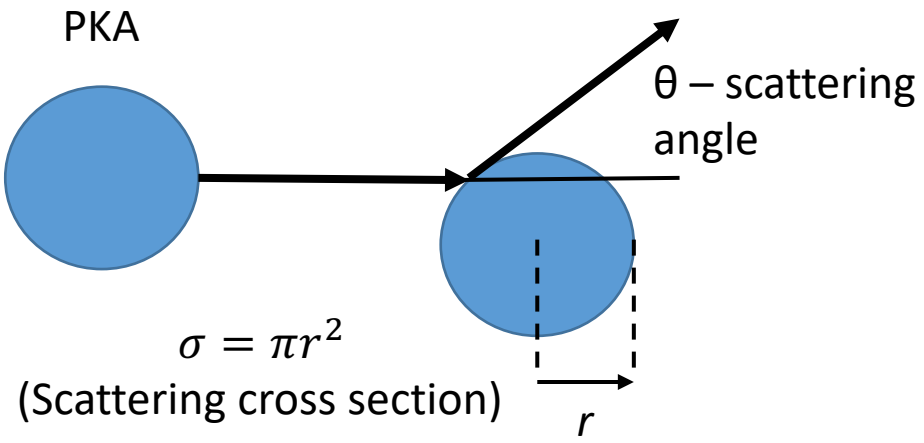
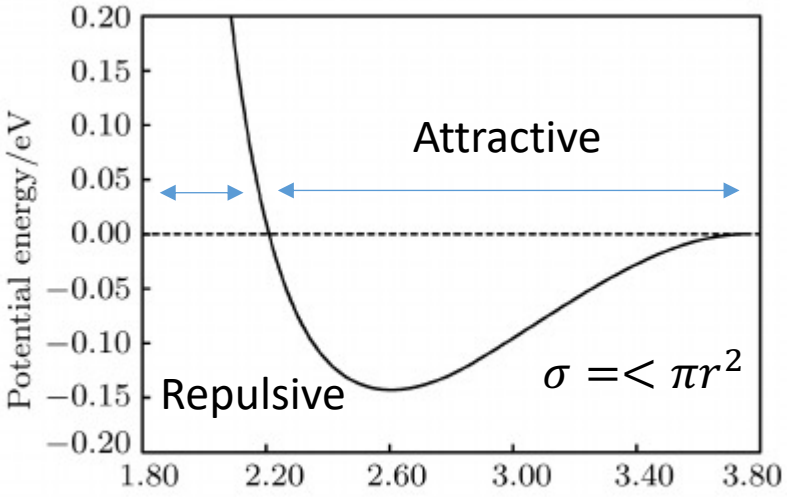



**Hard sphere model**




Interatomic distance /Å

# The NRT modified KP model

- Modifications of the KP model were made by Norgett, Robinson and Torrens (NRT) in 1975 - Still used in todays calculation of radiation damage in nuclear reactors!

- In reality there isn't a single cut-off for a PKA to lose energy to either atomic nuclei or electrons (so we need to take this into account for all energies)

- The hard-sphere model is a poor approximation and in reality atoms are not hard impenetrable shells – this overestimates the number of displacements caused!

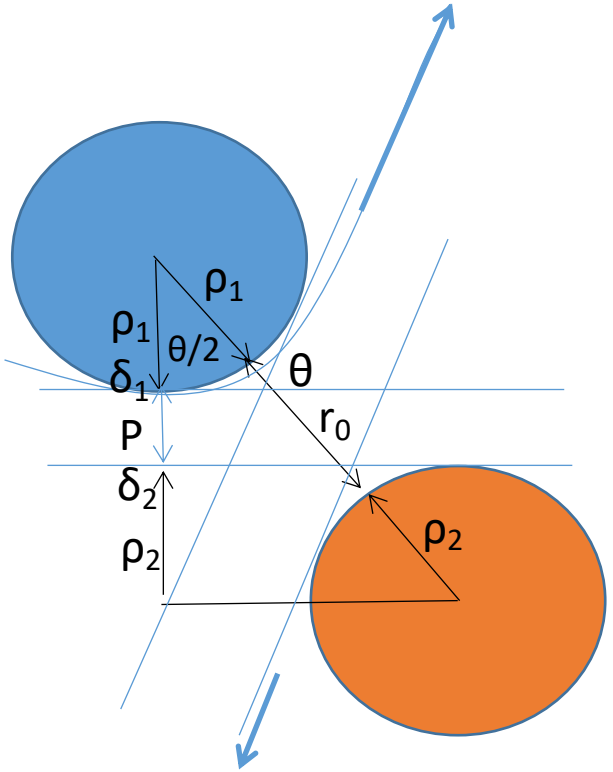
- NRT model proposed the following to the KP model;

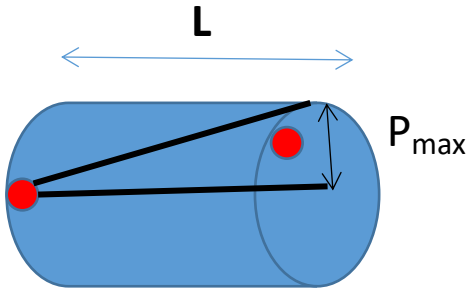
$$\nu(T) = \frac{T}{2E_d} \quad (\mathrm{KP}) \qquad\qquad \nu NRT(T) = \frac{k(T-Q)}{2E_d} = \frac{0.8(T_{dam})}{2E_d} \quad (\mathrm{NRT-KP})$$

- Where;
  - $k$ is the displacement efficiency (a constant given as 0.8) – accounts for decreased scattering cross-section compared to hard sphere approximation
  - $Q$ is the amount of energy lost to the electronic system (ionisation/excitation)
  - $T_{dam}$ is the energy available for displacements (i.e. minus electronic loss)

# SRIM damage calculation

- Monte Carlo two body elastic collisions (BCA)
  - No temperature effects
  - No crystallography effects
- Separates nuclear and electronic stopping
- Uses ‘magic formula’ to rapidly calculate the scattering angle and energy transfer
  - Solves θ from scattering triangle
  - $\frac{Cos\theta}{2} = \frac{\rho_1+\rho_2+\delta_1+\delta_2+P}{\rho_1+\rho_2+ro}$
  - δ correction factor for different Interatomic potentials
  - ~2% difference to values obtained from solving the scattering integral
- Uses a ‘free flight path’ of ion which also increased speed of calculation
  - Mean free path <<< distance between large angle scattering deflections >10°
  - SRIM checks that electronic energy loss per L is <5% (if not **L** is reduced)



# SRIM damage calculation

- ‘Ion distribution and Quick calculation of damage’ - KP calculation in SRIM doesn’t include replacement collisions

- ‘Detailed Calculation with Full Damage Cascades’ options in SRIM follow knock on atoms until they fall below a threshold energy and so does include replacements collisions

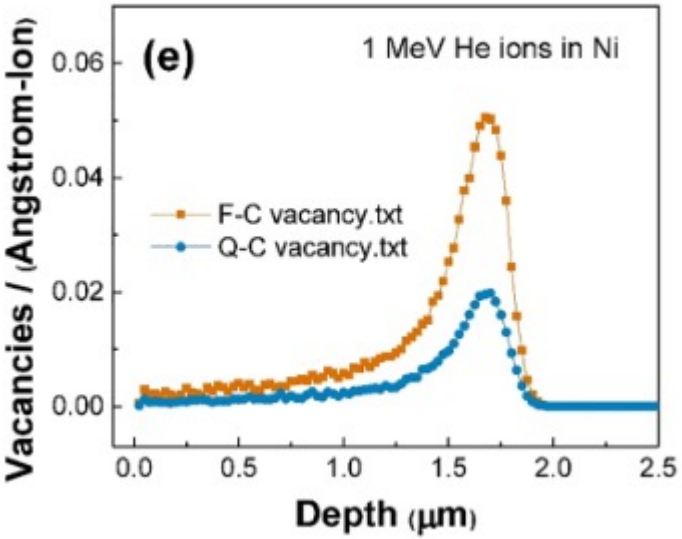



Figure from *Agarwal et al.* ***Nuc. Inst. Meth. Phys. Res. B, 503, 2021, 11-29***


Contents lists available at SciVerse ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb


On the use of SRIM for computing radiation damage exposure


R.E. Stoller [a,*], M.B. Toloczko [b], G.S. Was [c], A.G. Certain [b], S. Dwaraknath [c], F.A. Garner [d]

[a] Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, United States
[b] Pacific Northwest Laboratory, Richland, WA, United States
[c] Nuclear Engineering and Radiological Sciences, University of Michigan, Ann Arbor, MI, United States
[d] Radiation Effects Consulting, Richland, WA, United States



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On the use of SRIM for calculating vacancy production: Quick calculation and full-cascade options


S. Agarwal [a,*], Y. Lin [a], C. Li [a], R.E. Stoller [b], S.J. Zinkle [a,b]

[a] Department of Nuclear Engineering, University of Tennessee, Knoxville, TN 37996, USA

# Best Practice for Running SRIM

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1 – Run SRIM in 'Quick' Kinchin Pease option to 5000 ions

2 – Choose recommended $E_d$ from ASTM standard E521

3 – Set Lattice binding to 0 eV

4 – Compute $T_{dam}$ from;

$T_{dam}$ = Beam energy absorbed by target atoms – target atom energy lost to ionisation

5 – Calculate number of displacements;

$$v_{NRT}(T) = \frac{0.8(T_{dam})}{2E_d}$$

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[b] Materials Science & Technology Division, Oak Ridge National Lab, Oak Ridge, TN 37831, USA

1 – Run SRIM in 'Full Cascade' option to 10,000 ions

2 – Choose recommended $E_d$ from ASTM standard E521

3 – Set Lattice binding to 0 eV

4 – Compute $T_{dam}$ from;

$T_{dam}$ = Beam energy absorbed by target atoms – target atom energy lost to ionisation

5 – Calculate number of displacements;

$$v_{NRT}(T) = \frac{0.8(T_{dam})}{2E_d}$$

# Worked example

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**1 MeV He ions into Ni ($E_d$ = 40 eV)**

1 – Run SRIM in 'Full Cascade' option to 10,000 ions

2 – Choose recommended $E_d$ from ASTM standard E521

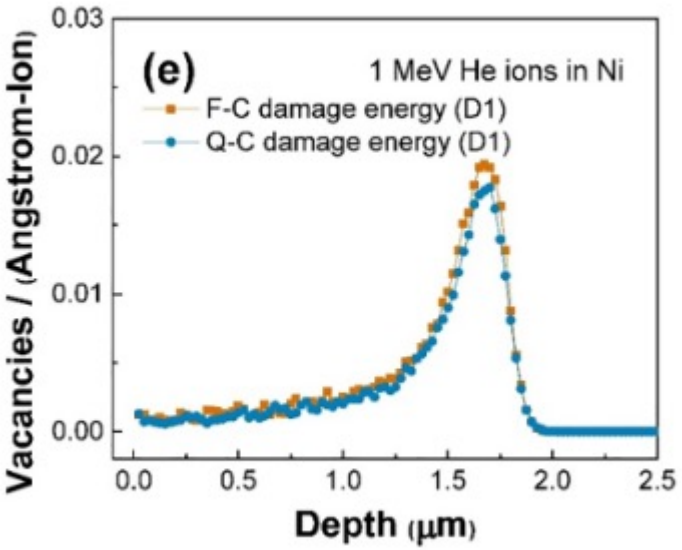
3 – Set Lattice binding to 0 eV

4 – Compute $T_{dam}$ from;

$T_{dam}$ = Beam energy absorbed by target atoms – target atom energy lost to ionisation

5 – Calculate number of displacements;

$$v_{NRT}(T) = \frac{k(T-Q)}{2E_d} = \frac{0.8(T_{dam})}{80}$$




| | |
|---|---|
| **E2recoil.txt** | Beam energy absorbed by target atoms |
| **Ionization.txt** | target atom energy lost to ionisation |

# Worked example

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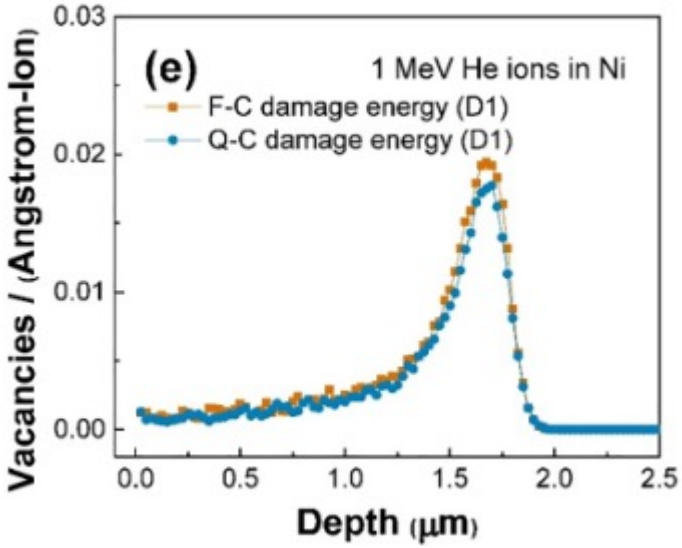
**How to calculate DPA from $V_{NRT}$**

**1 MeV He ions into Ni ($E_d$ = 40 eV)**




5 – Calculate number of displacements;

$$v_{NRT}(T) = \frac{0.8(T_{dam})}{2E_d}$$

6 – calculate displacements per atom (DPA)

$$DPA = \frac{ion\ fluence \times v_{NRT}}{Atomic\ density} = \frac{\frac{ions}{cm^2} \times \frac{vacancies}{ion.cm}}{\frac{Atoms}{cm^3}} = \frac{Vacancies}{Atom}$$

**(or NRT displacements!)**

# Worked example

Nuclear Instruments and Methods in Physics Research B 503 (2021) 11–29

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ARTICLE INFO

ABSTRACT

# (Future?) Best Practice for Running SRIM

nature COMMUNICATIONS

ARTICLE

DOI: 10.1038/s41467-018-03415-5 OPEN

## Improving atomic displacement and replacement calculations with physically realistic damage models

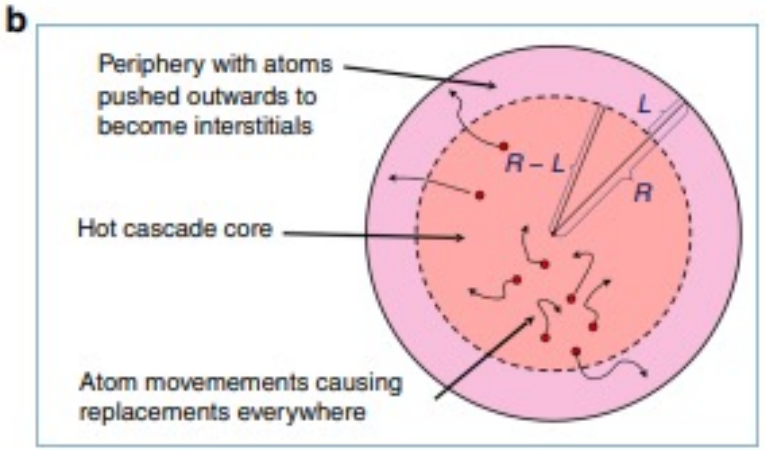
Kai Nordlund[1], Steven J. Zinkle[2,3], Andrea E. Sand[1], Fredric Granberg[1], Robert S. Averback[4], Roger Stoller[3], Tomoaki Suzudo[5], Lorenzo Malerba[6], Florian Banhart[7], William J. Weber[3,8], Francois Willaime[9], Sergei L. Dudarev[10] & David Simeone[11]

Replacements per atom (RPA) – term to understand the amount of in-cascade mixing due to energetic displacement cascades

Number of surviving defects from radiation damage in high energetic irradiated metals ~1/3 of the NRT model

Athermal recombination corrected (ARC-)DPA

Considers in-cascade recombination and thus reduction in vacancy production rate



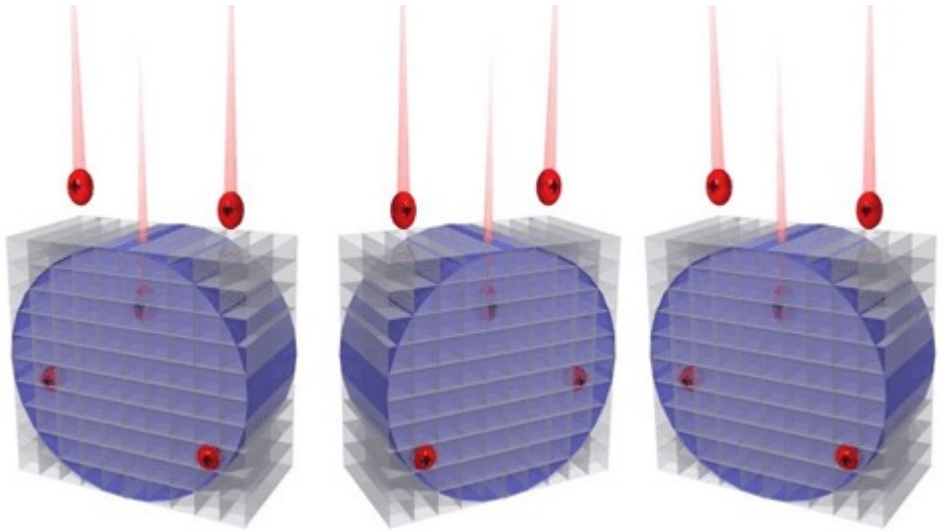

Nordlund et al. Nat. Comms., 9, 2018, 1084

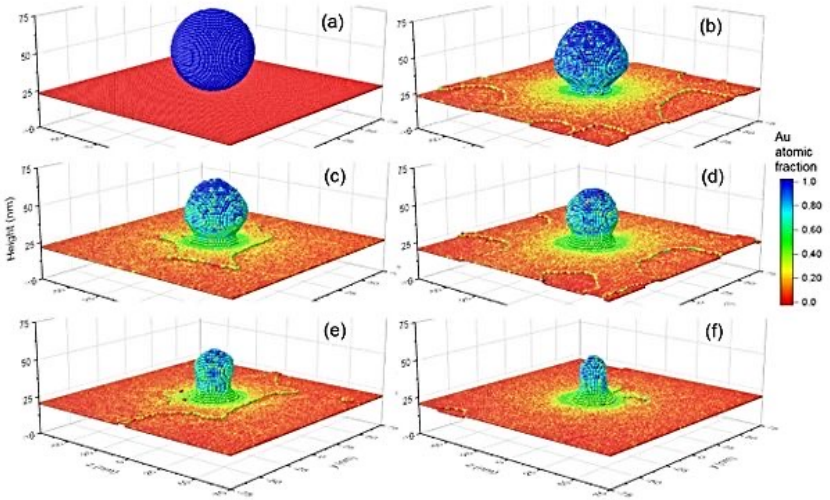
# Other BCA codes for 3D ion beam irradiation

- Irradina code offers the ability to perform irradiation 3-D structures
  - Unlike SRIM flat/bulk targets

- It works very similarly to SRIM
  - BCA-MC transport algorithm
  - No temperature effects
  - No crystallographic effects
  - Uses lookup tables instead of calculating scattering angles/energy transfers

- TRIDYN
  - TRI3DYN will allow dynamic change of the target composition due to radiation damage






H. Holland-Moritz et al., Semicond. Sci. Tech. 30(2015)33001

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# Best practice for SRIM radiation damage calculations

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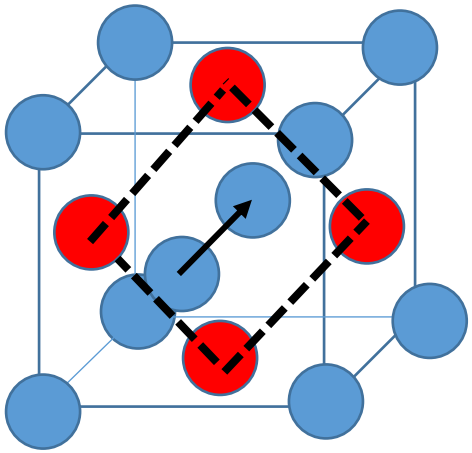
# Backup slides

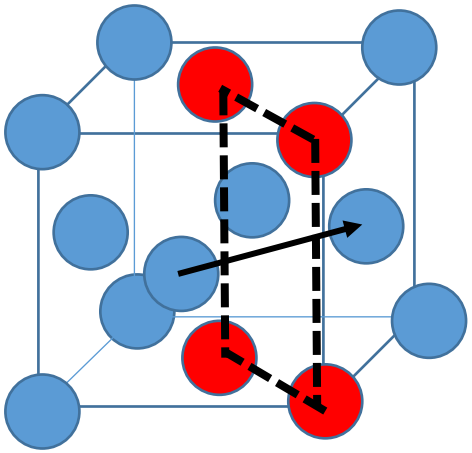
# Displacement energy ($E_d$)

- Often quoted a single value for calculations
- But there are minimum and maximum ranges of $E_d$ due to;
  - **Crystallographic effects**
  - The thermal energy in the lattice atom
- Consider displacing an atom in a face centred cubic (FCC) material and the barriers atoms it faces to displacement in that direction



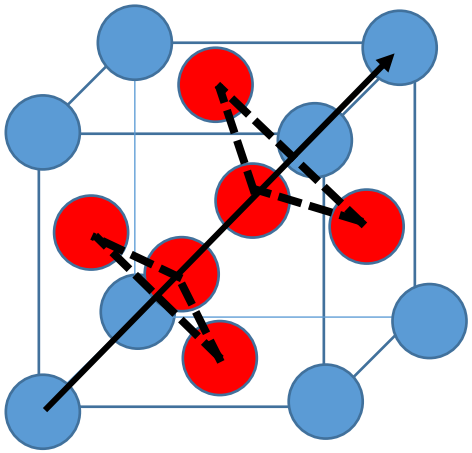
<100>

$E_d$ Cu = 19 eV



<110>

$E_d$ Cu = 23 eV

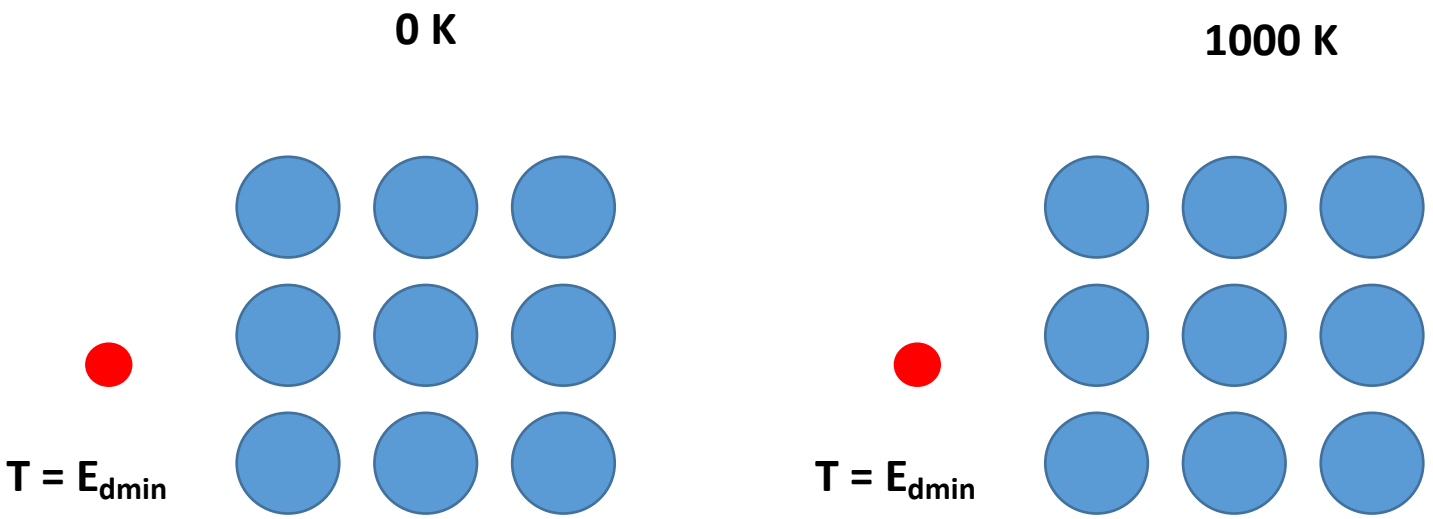


<111>

$E_d$ Cu = 76 eV

# Displacement energy ($E_d$)

- Often quoted a single value for calculations
- But there are minimum and maximum ranges of $E_d$ due to;
  - Crystallographic effects
  - **The thermal energy in the lattice atom**



# SRIM damage calculation

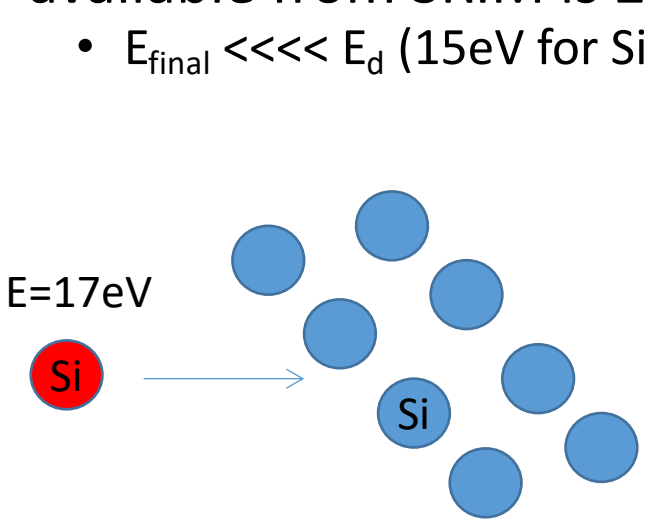
- Full cascade model includes replacements collisions which occur in SRIM when;

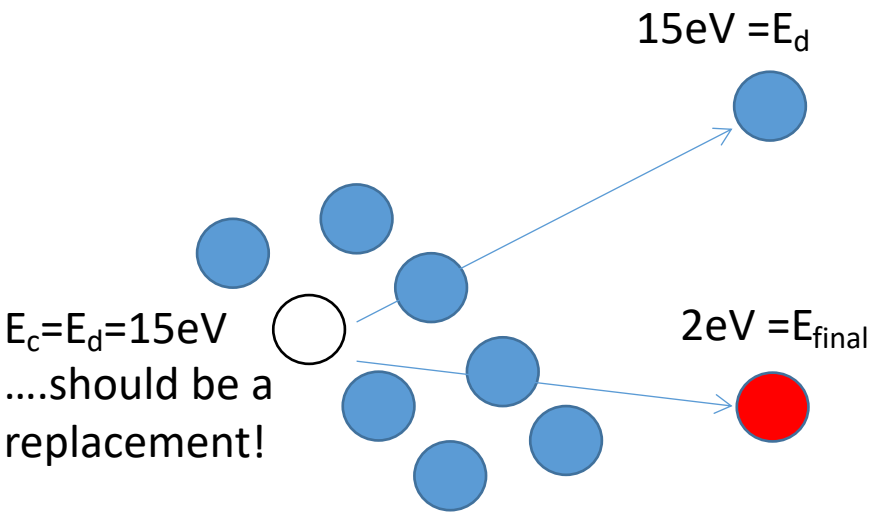
**(1)** The moving atom must be identical to the target atom.

**(2)** The incident atom must end with less energy than $E_{final}$ (it must stop).

**(3)** The struck atom must have enough energy to move on, i.e. its energy is greater than $\mathbf{E_{disp}}$.

- However, $E_{final}$ cannot be altered by the user and the only figure available from SRIM is 2eV for Si
  - $E_{final}$ <<<< $E_d$ (15eV for Si)




- Therefore FC underestimates the number of replacement collisions thus overestimates vacancies!