Modifications to K-P Displacement Model & Stopping Powers

K.G. Field[1,a],
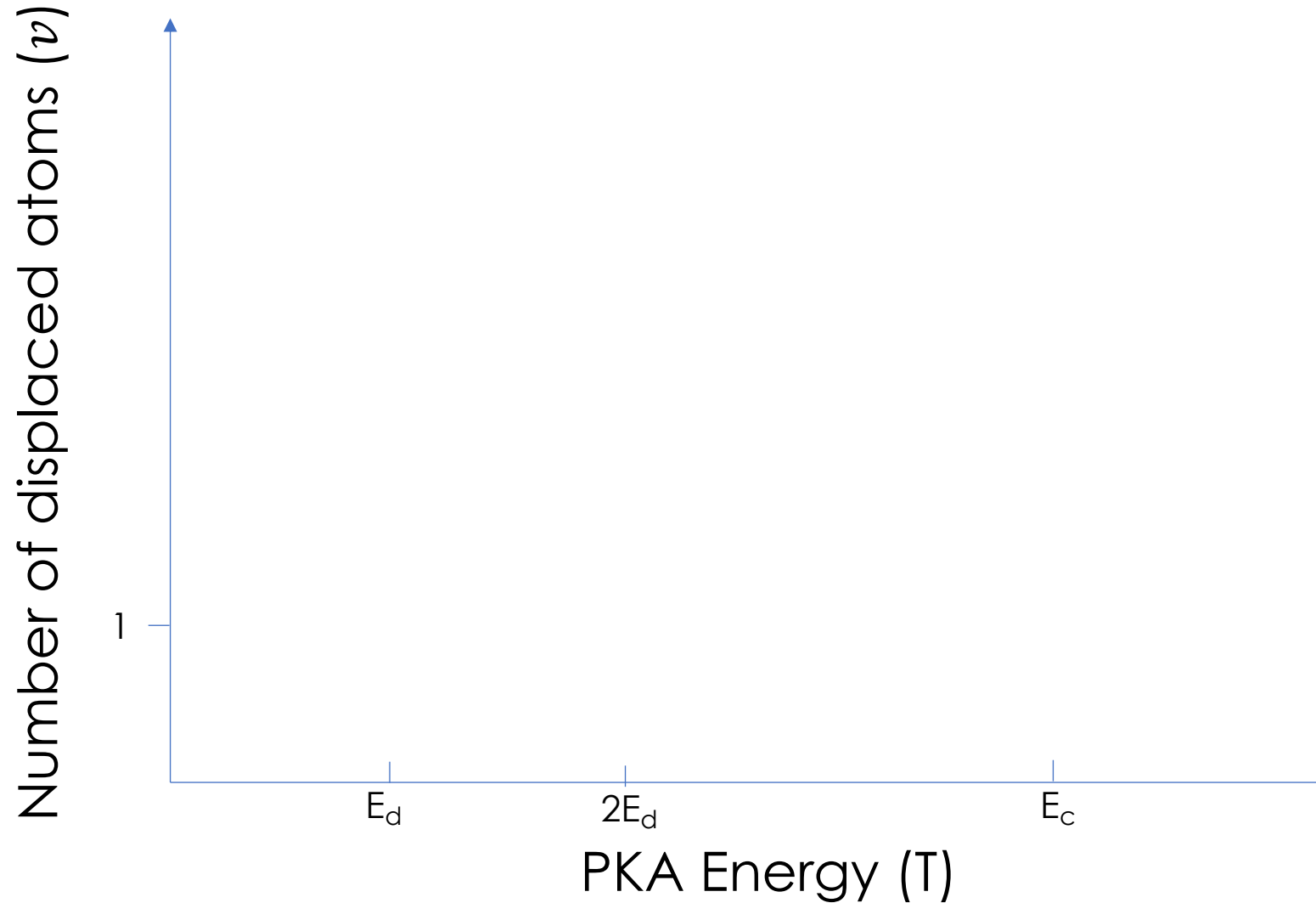
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Summary of Topics Covered

Outline

Stopping Powers:
- Remember E_C
- Concept of stopping power
- Regimes of electronic energy loss
- Compare electronic and nuclear stopping

Modifications of K-P Model:
- Accounting for electronic energy loss
- Effects of crystallinity
- NRT model + Arc-dpa model

Goal: Understand the concept of stopping power and how different physics modifies the displacement model

A simple picture of slowing down

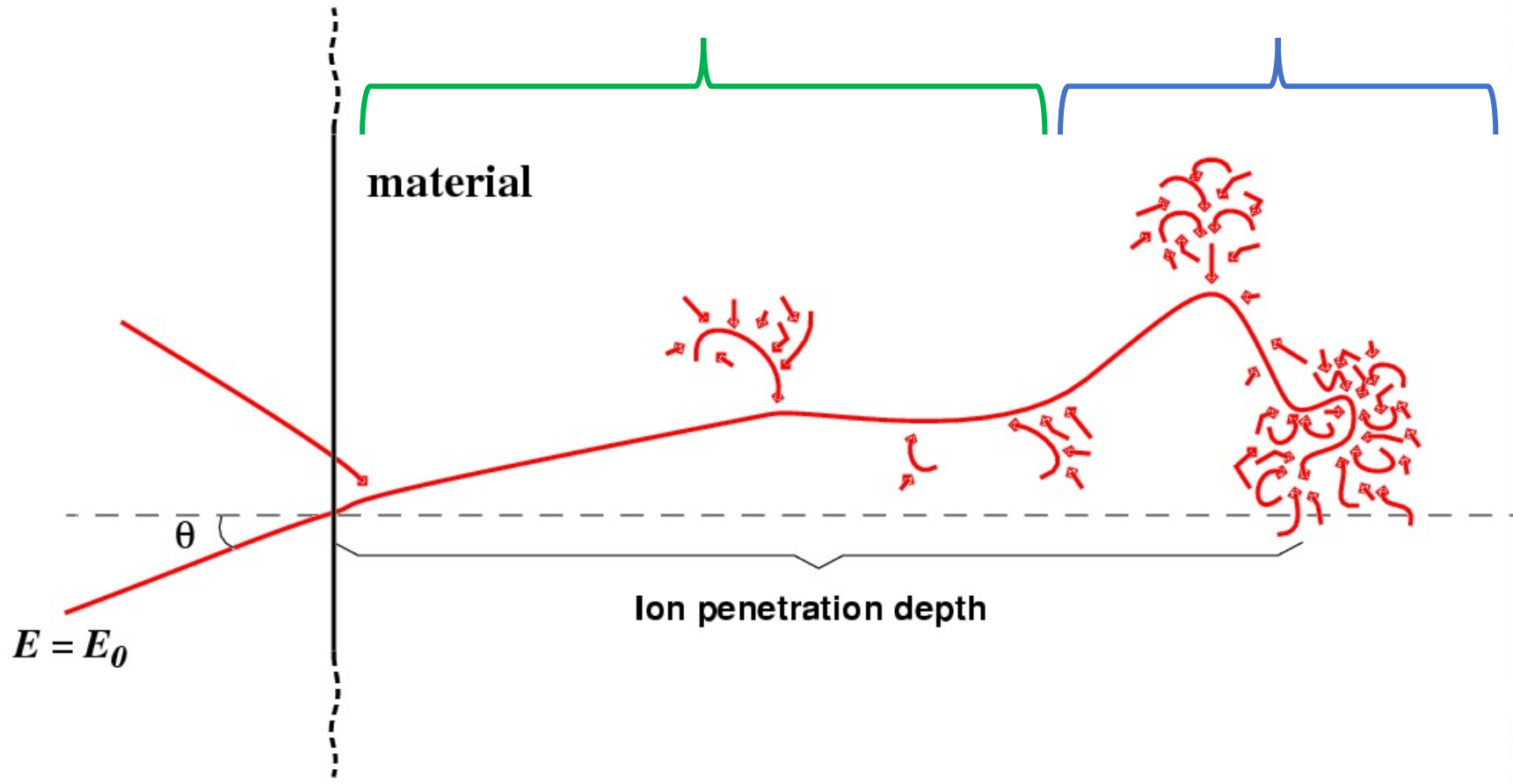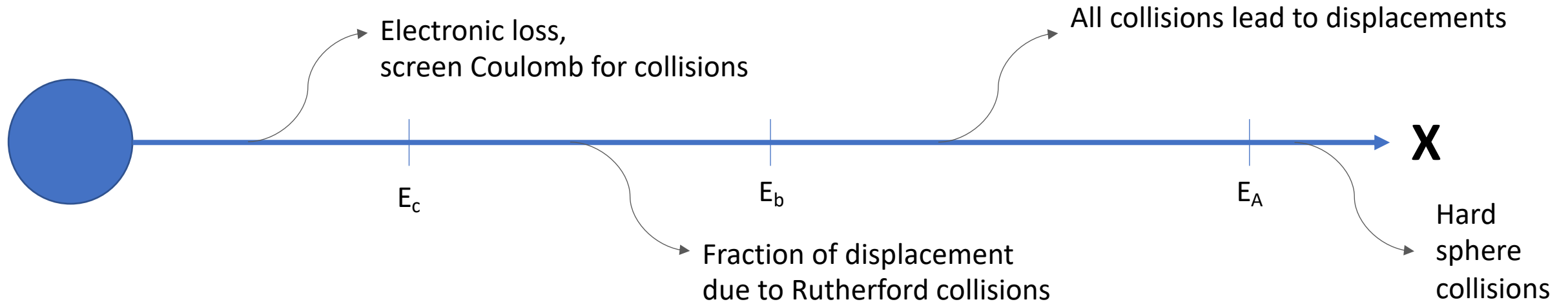- The slowing down process of an ion impacting on a surface:

Image: Kai Nordlud

Regimes of energy loss of a PKA

The concept of stopping power

- Since the electronic collisions only slow down the ion, and the number of collisions is at high energies large, the effect of the electrons can be considered to be an average frictional force slowing down the ion

- This is known as the **electronic stopping power**

- The collisions with ions can also be averaged and then considered a **nuclear stopping power**

- The nuclear reactions can also be averaged and considered a **nuclear reaction stopping power**

material

θ

$E = E_0$

Ion penetration depth
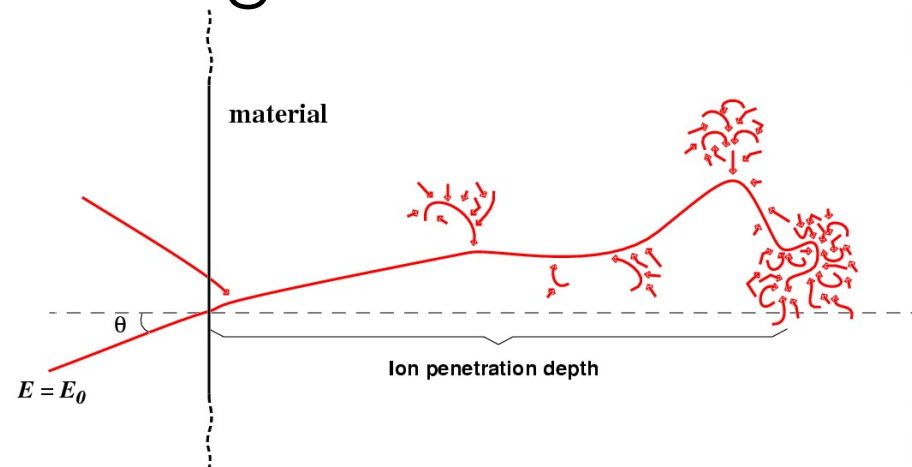
Stopping power

- The total stopping power can be written as

- Schematically, the energy dependence of these is then:
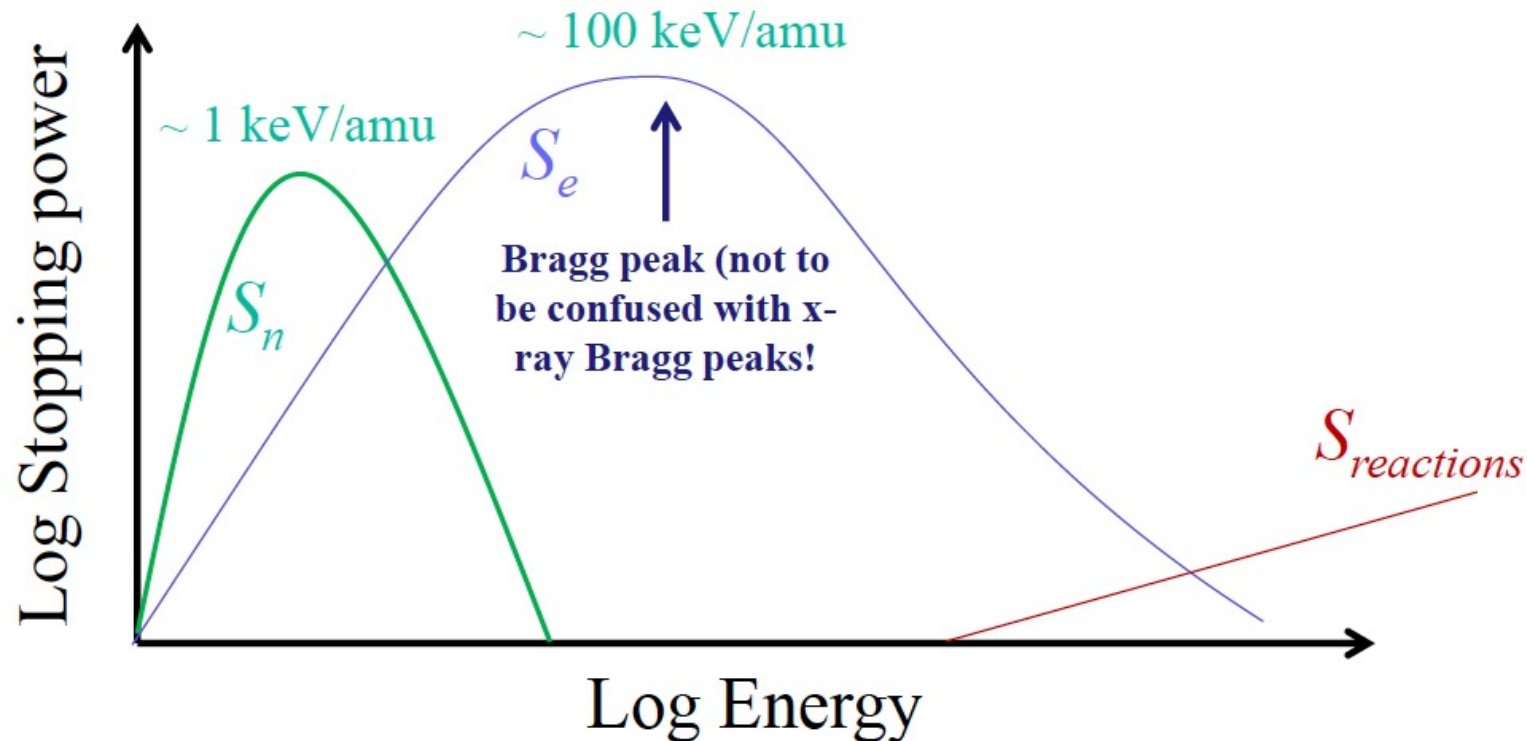
Stopping power

- The total stopping power can be written as

- Sche

Terminology Notes:

- In detector and space physics different terms are used:
- Linear Energy Transfer (LET) is used for total or **electronic stopping power**
- Total and electronic are about the same in this field due to the high energies (MeV and GeV)
- Non-ionizing energy loss is used for **nuclear stopping power**
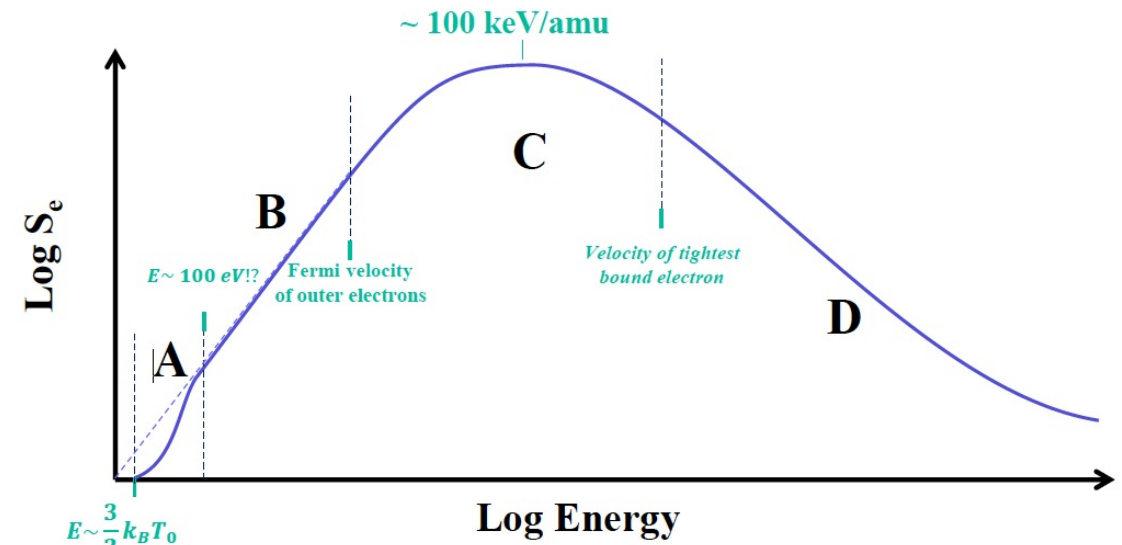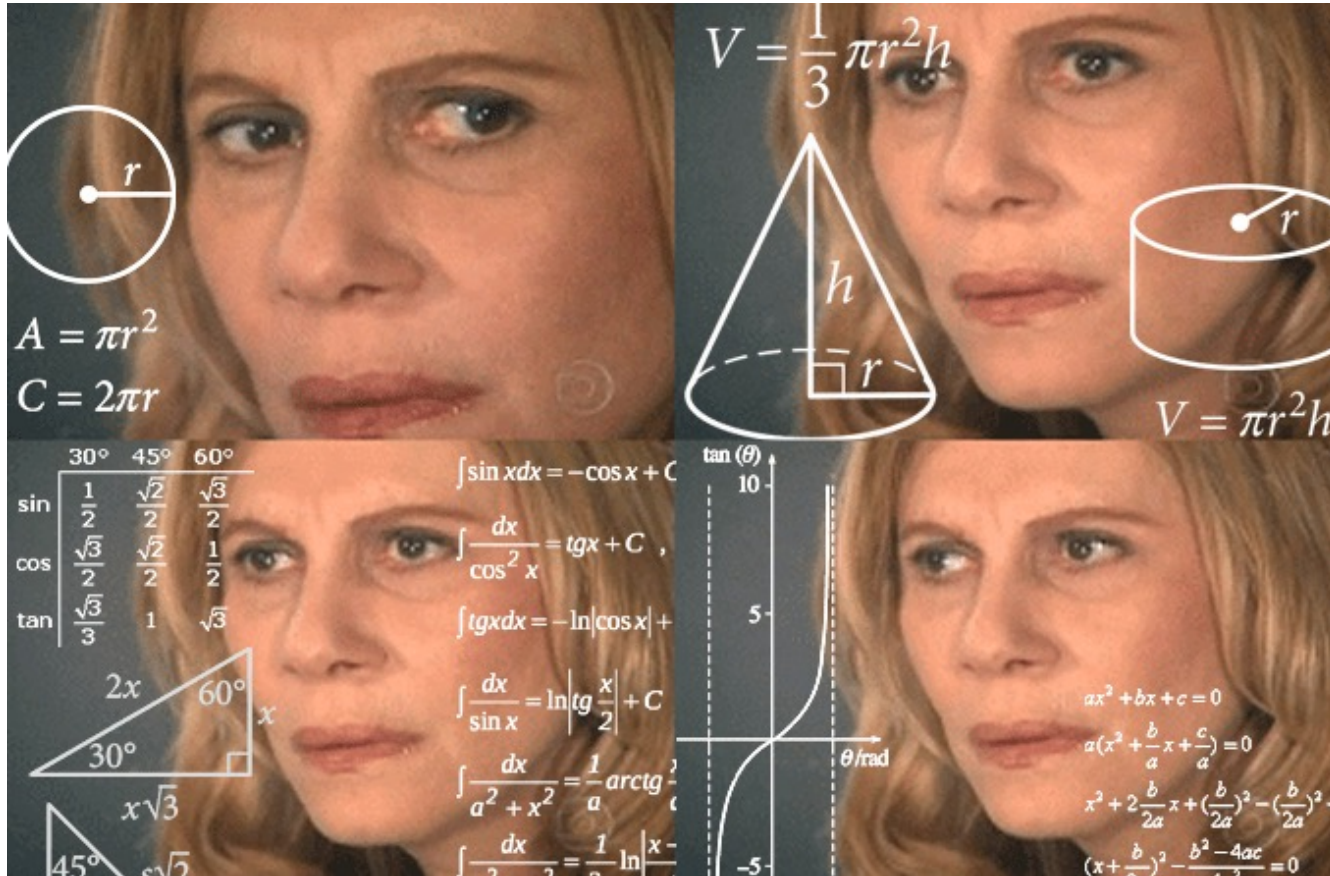
Log Energy

Regimes of electronic stopping power

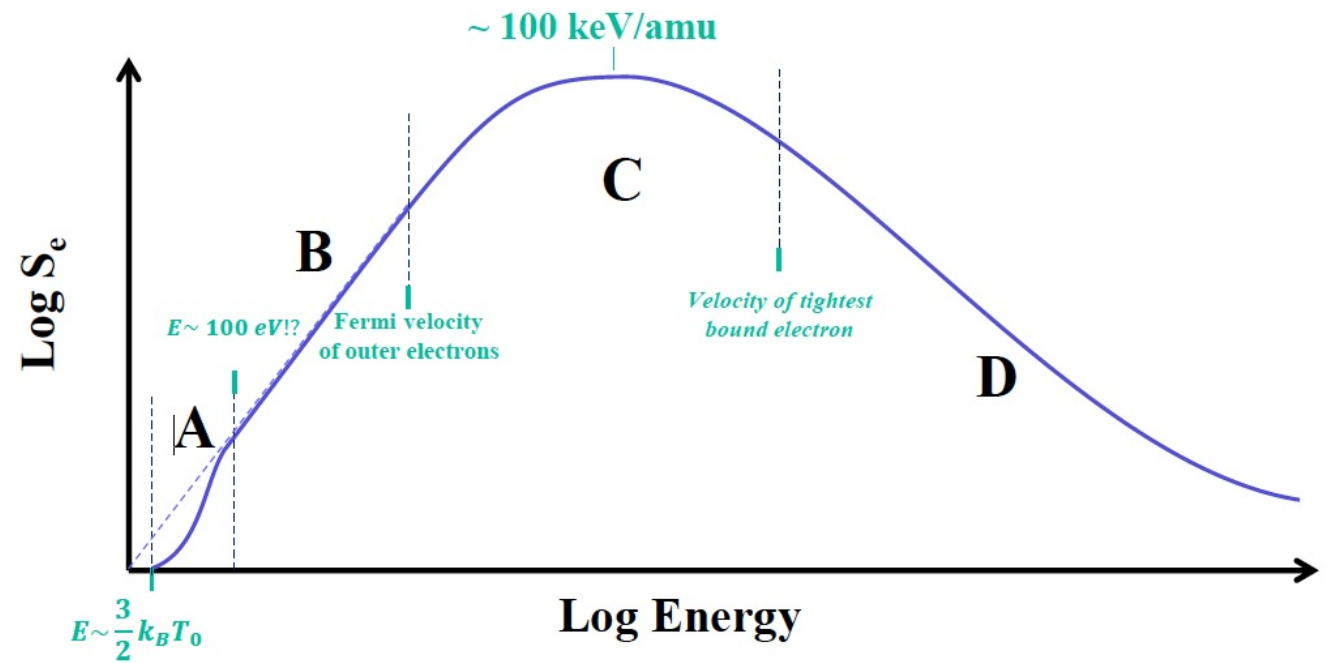• Electronic stopping can be segregated into four primary regimes:
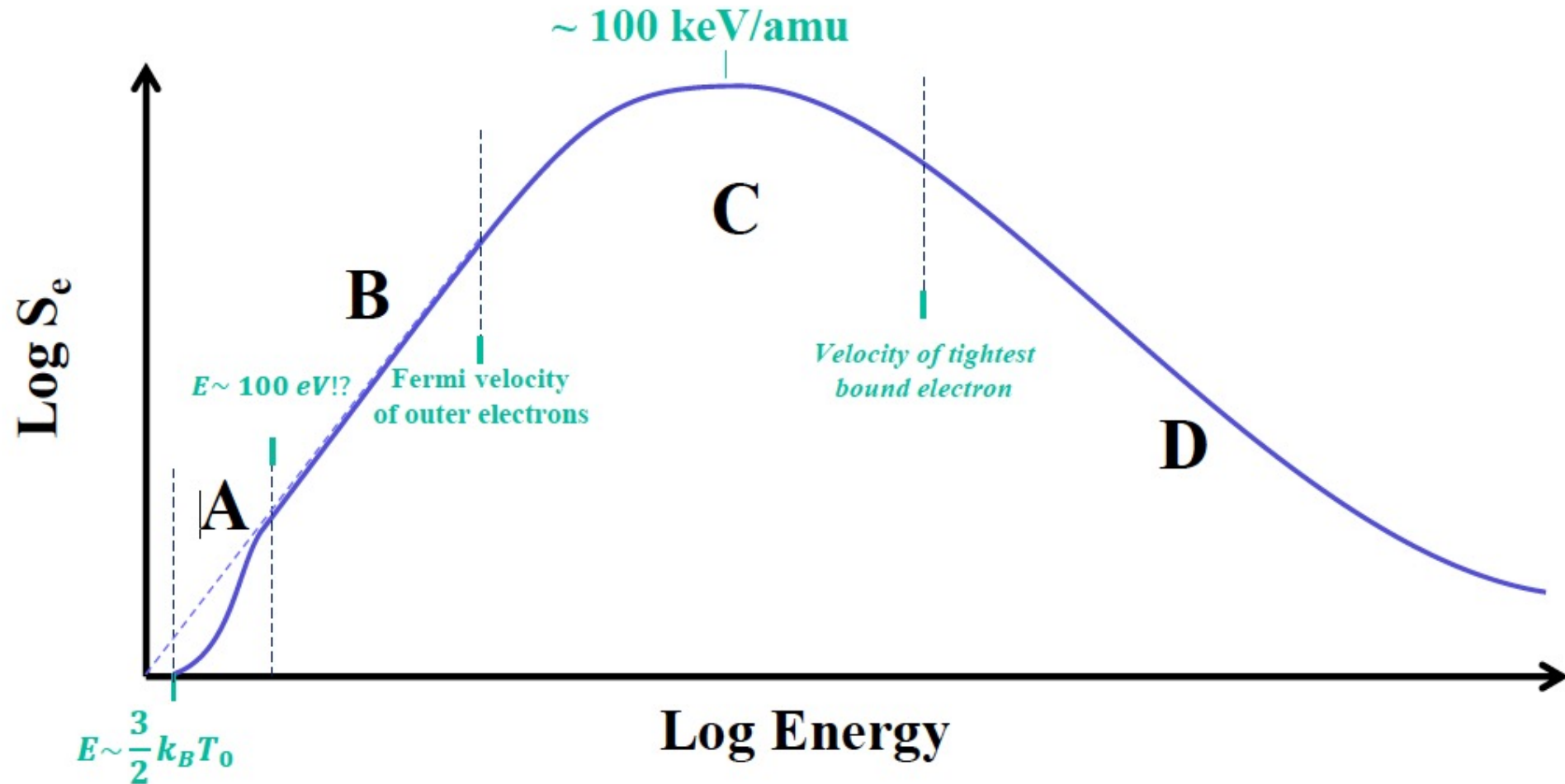
Regime A: low energy regime

The lowest energy regime is the least well known without simple analytical forms

Regime B: LSS theory

- At higher energies than region A the stopping is almost perfectly linear to the ion velocity,

- This regime has an upper limit at the Fermi velocity of the outermost electron of the material

- Regime and derivations agree well with experiments

Regime C:
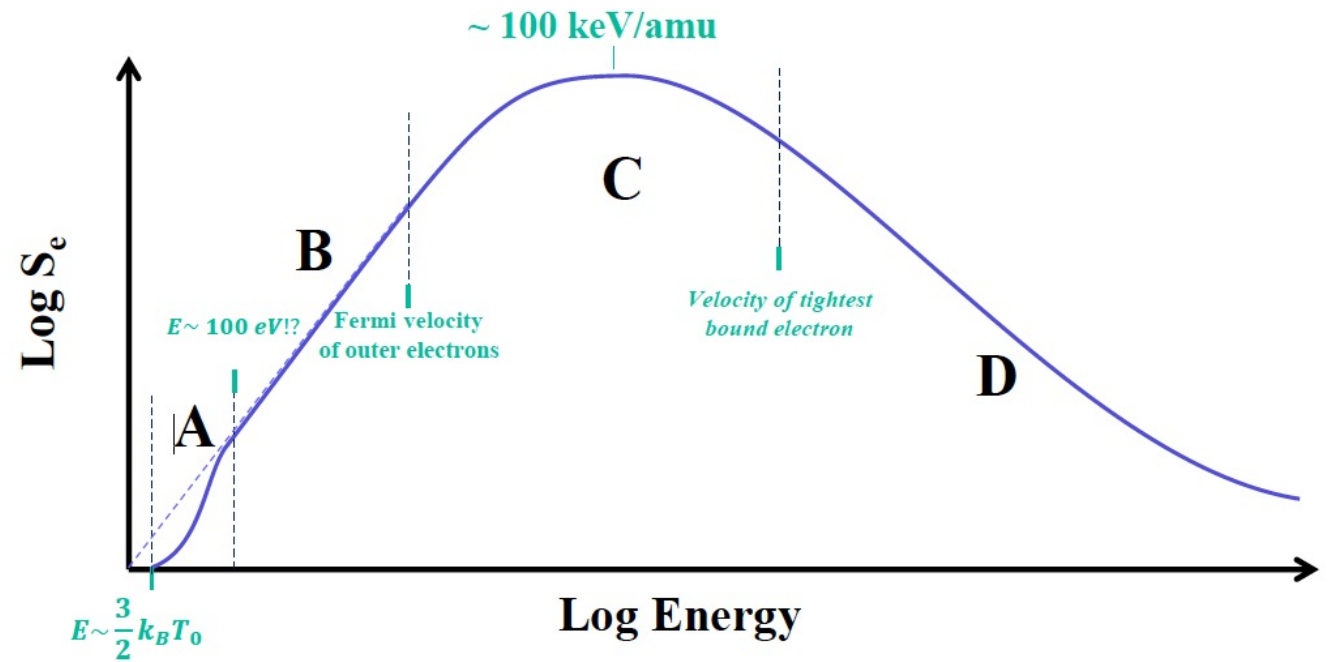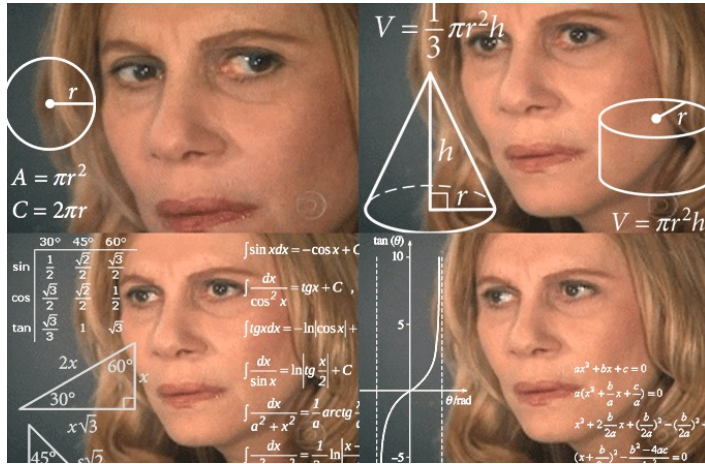
- The maximum region in the stopping power is a regime where the moving ion is partly ionized, and its charge state fluctuates
- I.e. it undergoes stochastic charge exchange processes with the atoms of the material
- There is no simple analytical equation that can describe this region fully reliably

Regimes of D: Bethe-Bloch

- The highest-energy regime can be well understood based on the Bethe-Bloch theory, derived already in the 1930's

- At these high energies, the moving ion is fully or highly charged and does not change charge state

- The Bethe-Bloch equations derive the stopping power quantum mechanically for a charged particle moving in a homogeneous electron gas
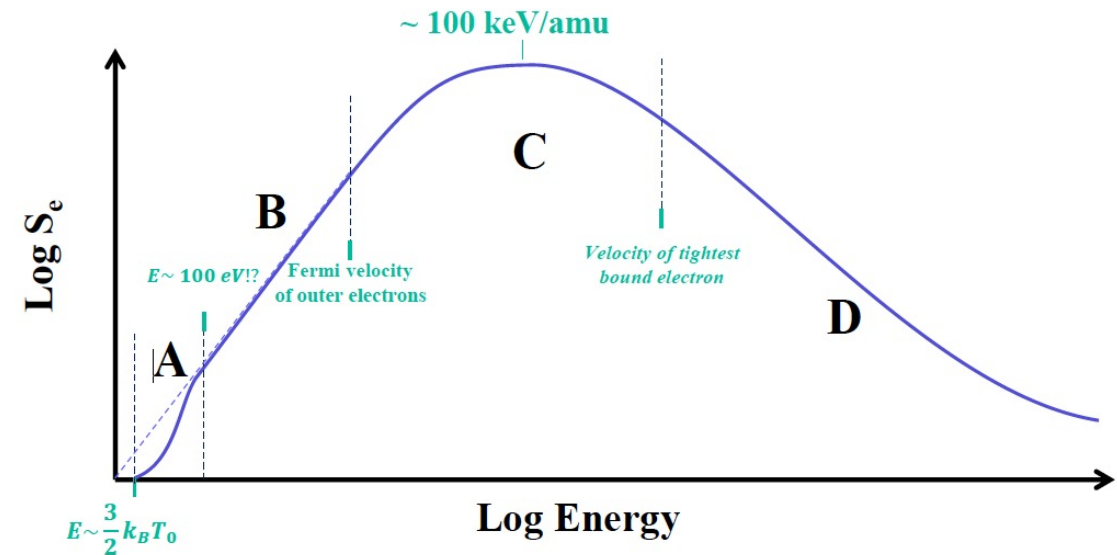
$$\left(-\frac{dE}{dx}\right)_e = \frac{N2\pi Z_1^2 Z_2 \varepsilon^4}{E_i}\frac{M}{m_e}\ln\left(\frac{\gamma_e E_i}{\bar{I}}\right) = \frac{2\pi N Z_1^2 M \varepsilon^4}{m_e E_i}B \qquad B = Z_2\ln\left(\frac{\gamma_e E_i}{\bar{I}}\right)$$

Energy Loss & Stopping

Stopping powers

- $\left(-{}^{dE}/_{dx}\right)_{total}$ can be written in terms of stopping power (units of energy * distance^2):

- Nuclear:

- Electronic:

Relative Stopping Powers
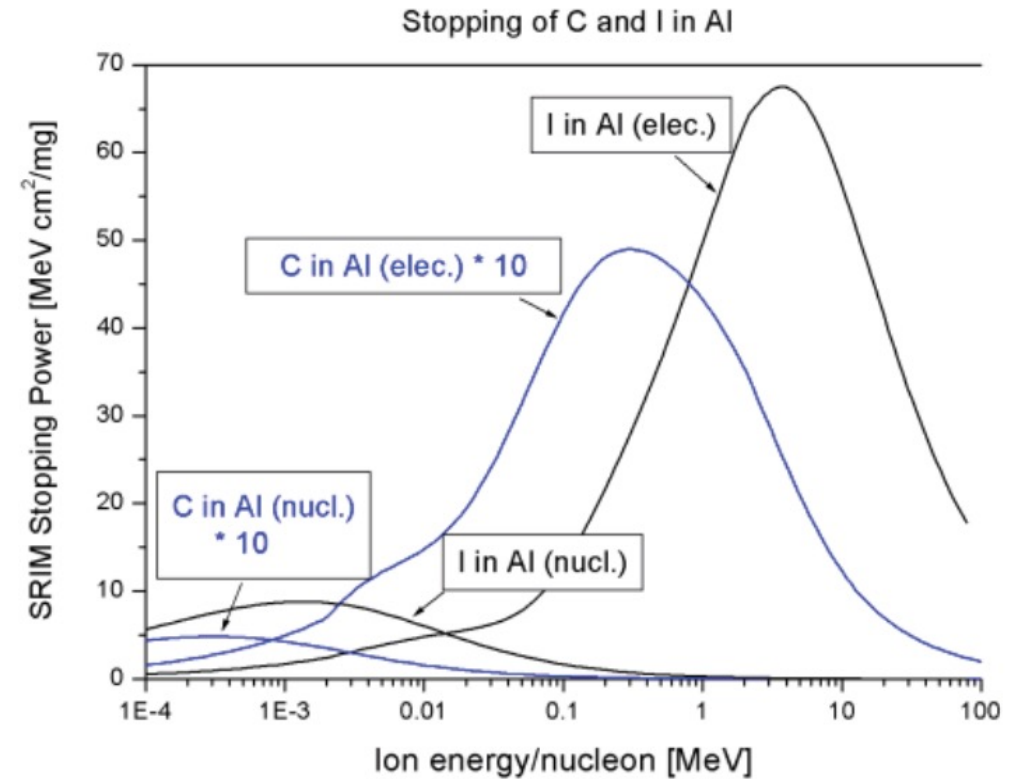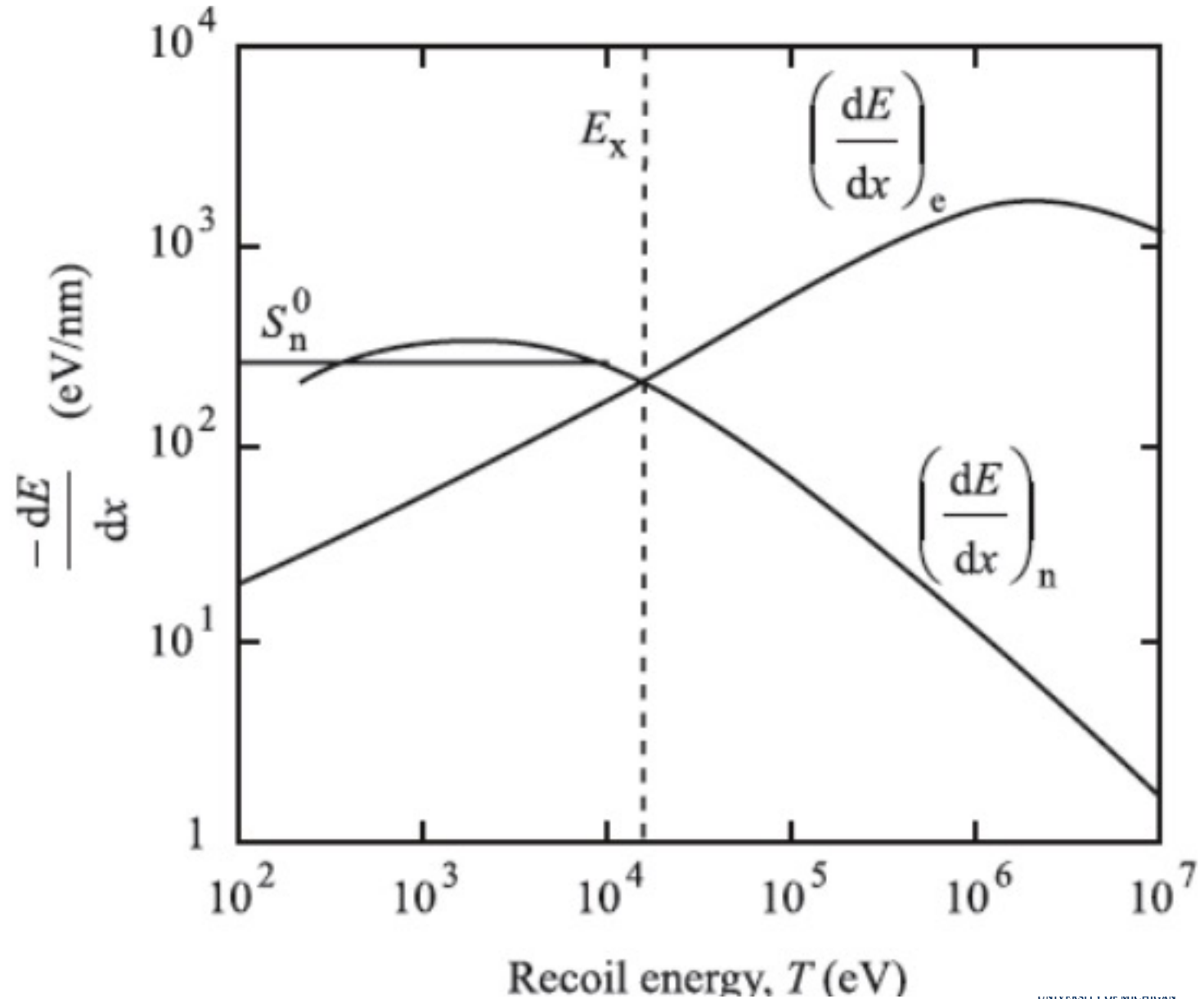
- Compare S_e/S_n:

Stopping of C and I in Al

FIGURE 2. Electronic and nuclear mass stopping power for carbon and iodine ions in aluminum, calculated using SRIM.

- Electronic stopping power dominates for high energy ions

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Relative Stopping Powers

Stopping powers

Table 1.7 Summary of energy loss rates for various types of interactions

| Type of interaction	Nuclear energy loss rate $\left(-\dfrac{dE}{dx}\right)_n$		Electronic energy loss rate $\left(-\dfrac{dE}{dx}\right)_e$	
High E Coulomb	$\dfrac{4N\pi Z^4 a_0^2 E_R^2}{E_i}\ln\left(\dfrac{a^2 c^2 E_i^2}{4a_0^2 E_R^2 Z^4}\right)$	(1.134)	$N\pi\dfrac{Z_1^2 Z_2 \varepsilon^4}{E_i}\dfrac{M}{m_e}\ln\left(\dfrac{\gamma_e E_i}{\bar{I}}\right)$	(1.173)
Low E	General expression: $\dfrac{8.462 \times 10^{-15} NZ_1 Z_2 M_1 S_n(\in)}{(M_1 + M_2)(Z_1^{0.23} + Z_2^{0.23})}$	(1.169)	$k' E_i^{1/2}$ $k' = 3.83\dfrac{Z_1^{7/6} Z_2}{M_1^{1/2}\left(Z_1^{2/3} + Z_2^{2/3}\right)^{3/2}}$	(1.178) (1.179)
	Inverse square: $\dfrac{\pi^2}{4}a^2 NE_a\gamma$	(1.159)	$k E_i^{1/2}$	(1.190)
	Thomas–Fermi screening: $K\dfrac{NZ_1 Z_2}{Z^{1/3}}\dfrac{M_1}{M_1 + M_2}$ where $Z^{1/3} = \left(Z_1^{2/3} + Z_2^{2/3}\right)^{1/2}$ and $K = \left(\dfrac{\pi}{e}\right)\varepsilon^2 a_0 = 2.8 \times 10^{-15}\ eV \cdot cm^2$	(1.163)	$k = 8\sigma_e N\left(\dfrac{m_e}{M_1}\right)^{1/2}$ valid for $0 < E\,(keV) < 37Z^{7/3}$	

Lecture Break

- In October 1997, the Thrust SSC achieved the current land speed record by traveling how fast in the Black Rock Desert, Nevada, USA?
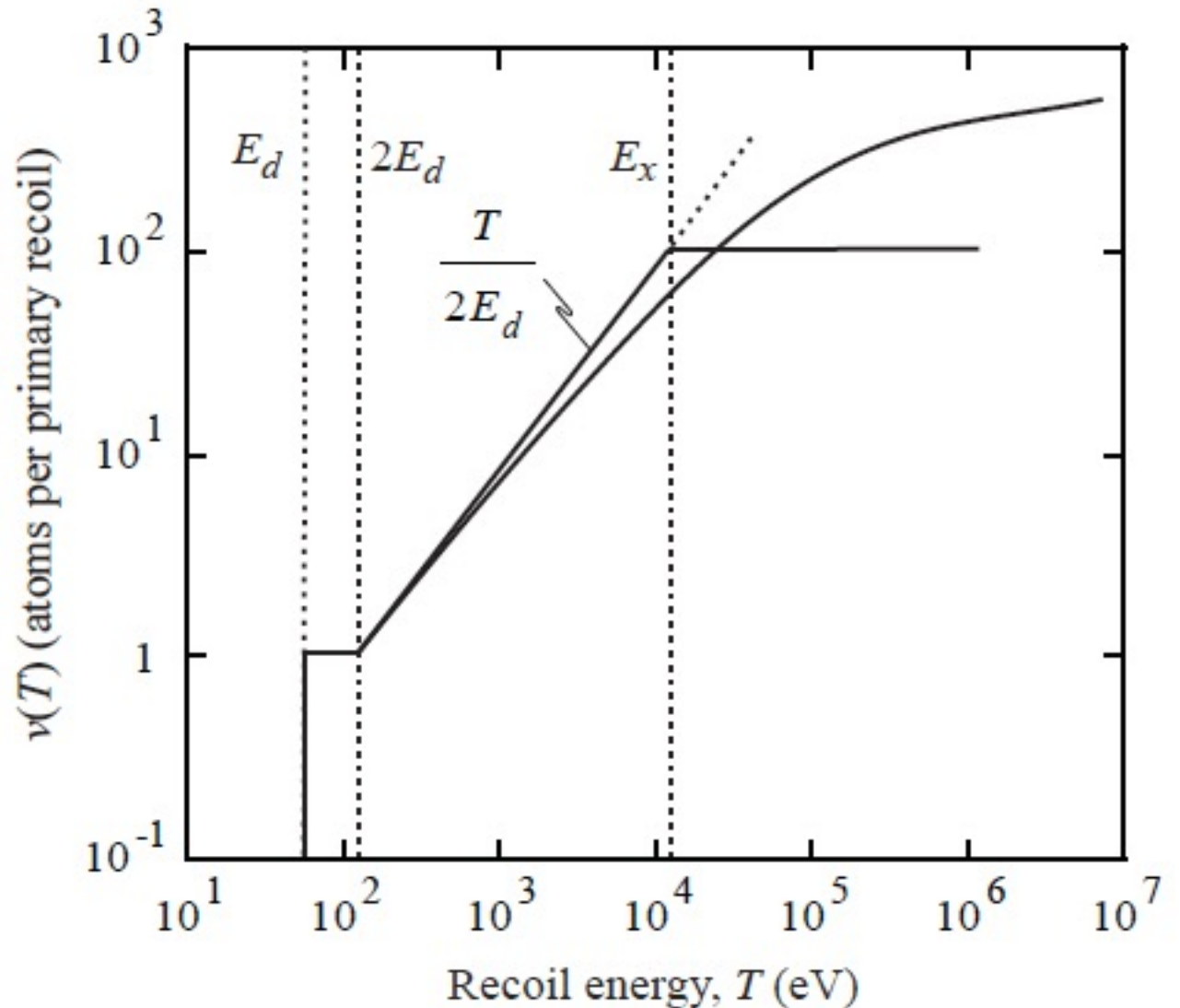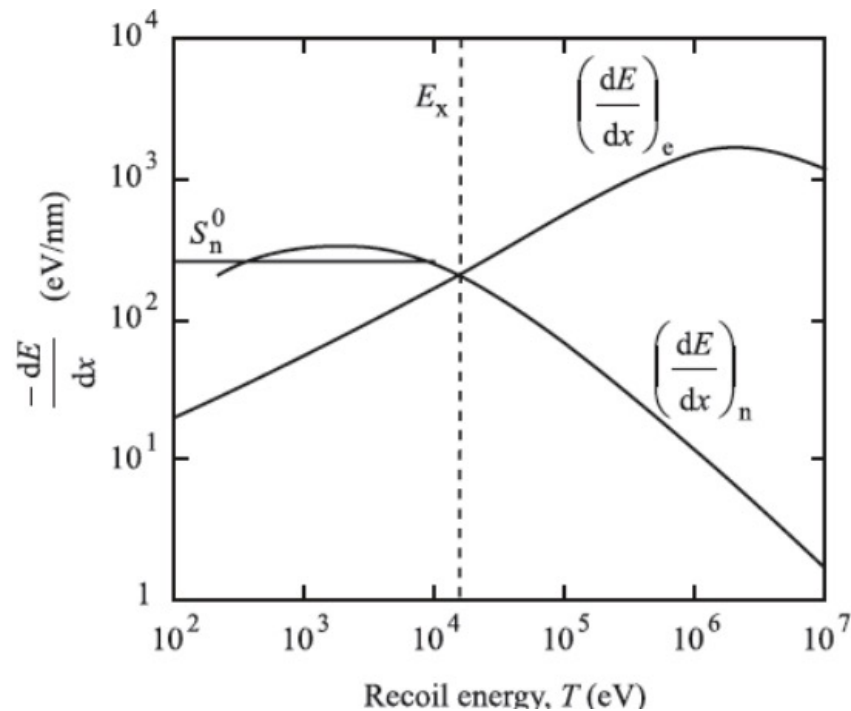
Modifications to K-P Model

- Many factors to consider (and covered in text), but three are the most important:
  1. Correction for electron energy loss
  2. Use of a realistic cross-section
  3. Effect of crystallinity
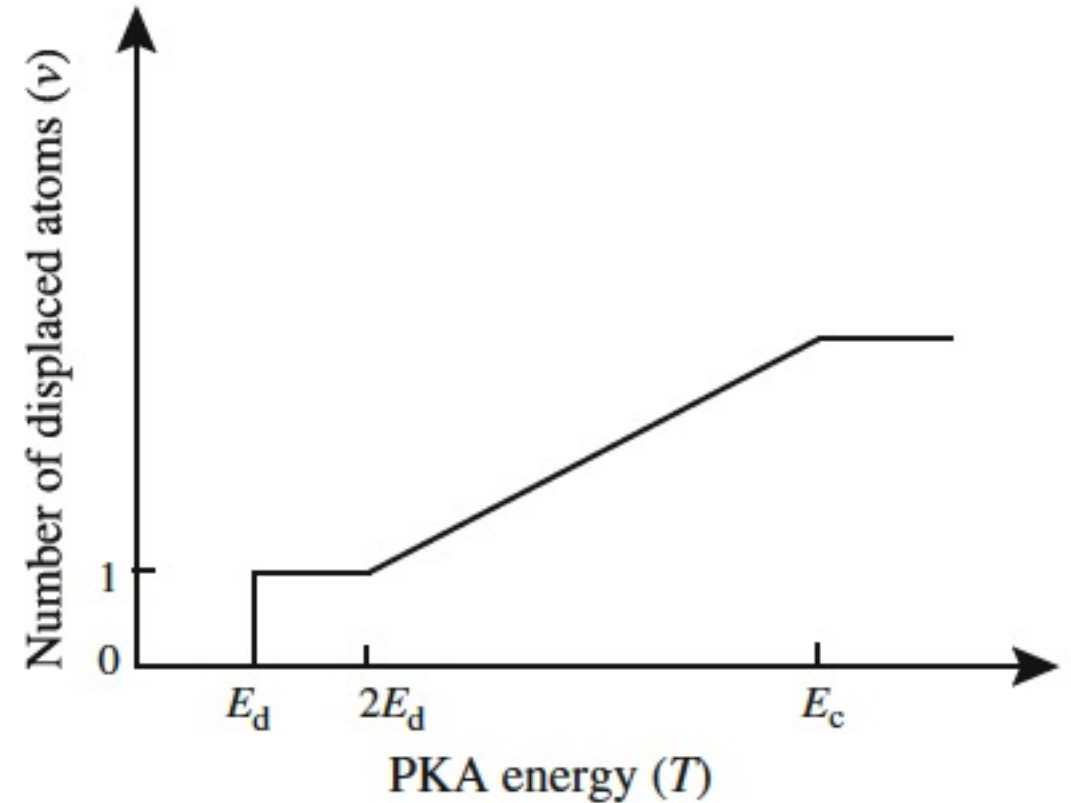
Modifications to K-P Model
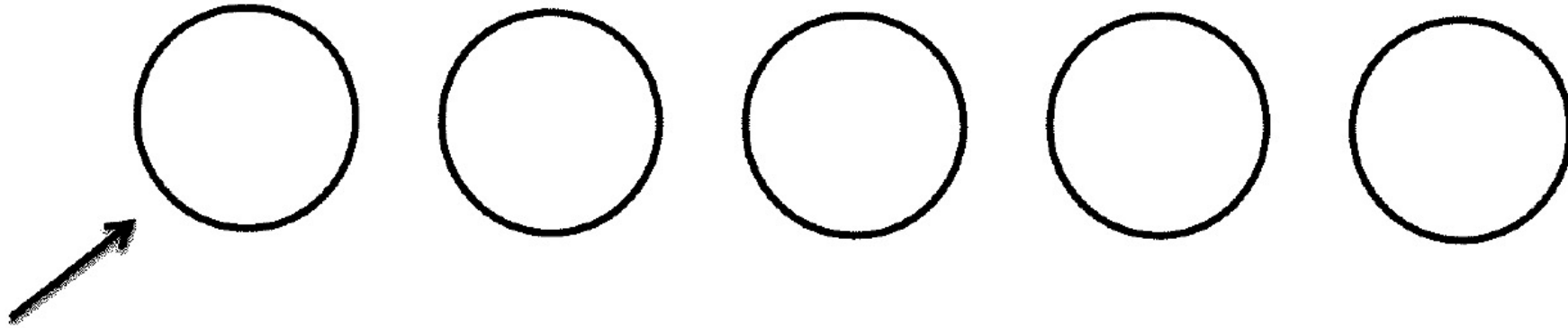
1. Correction for electron energy loss
   - Nuclear power diminishing above E_c but does not disappear
   - Electronic stopping starts before E_c

Modifications to K-P Model

2.   Use of realistic cross sections

A simple thought experiment

To the document reader!

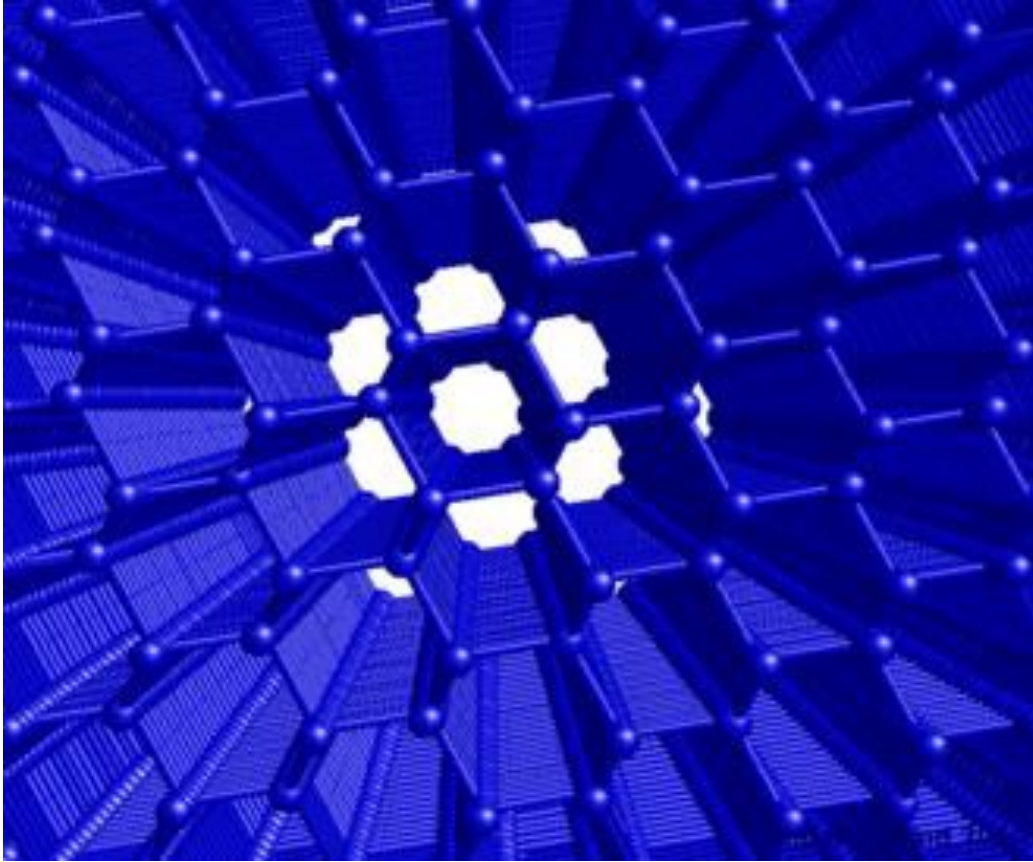# Modifications to K-P Model

3. Effect of crystallinity:

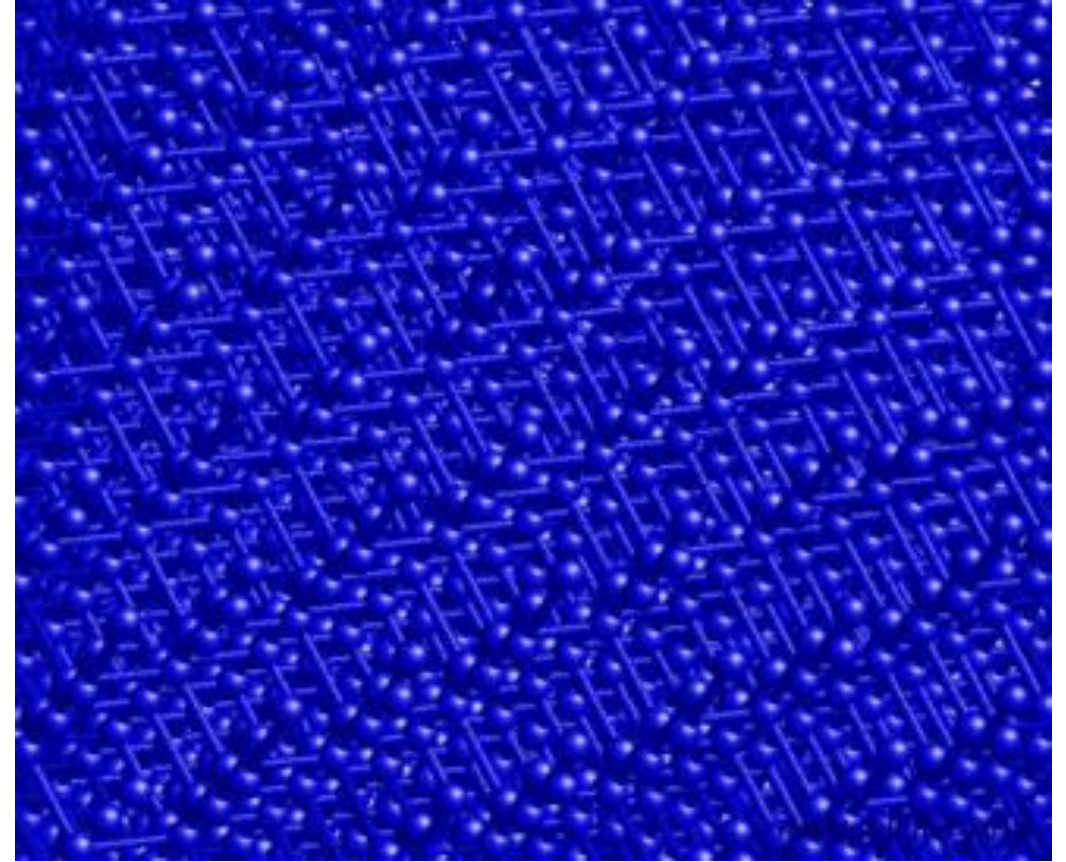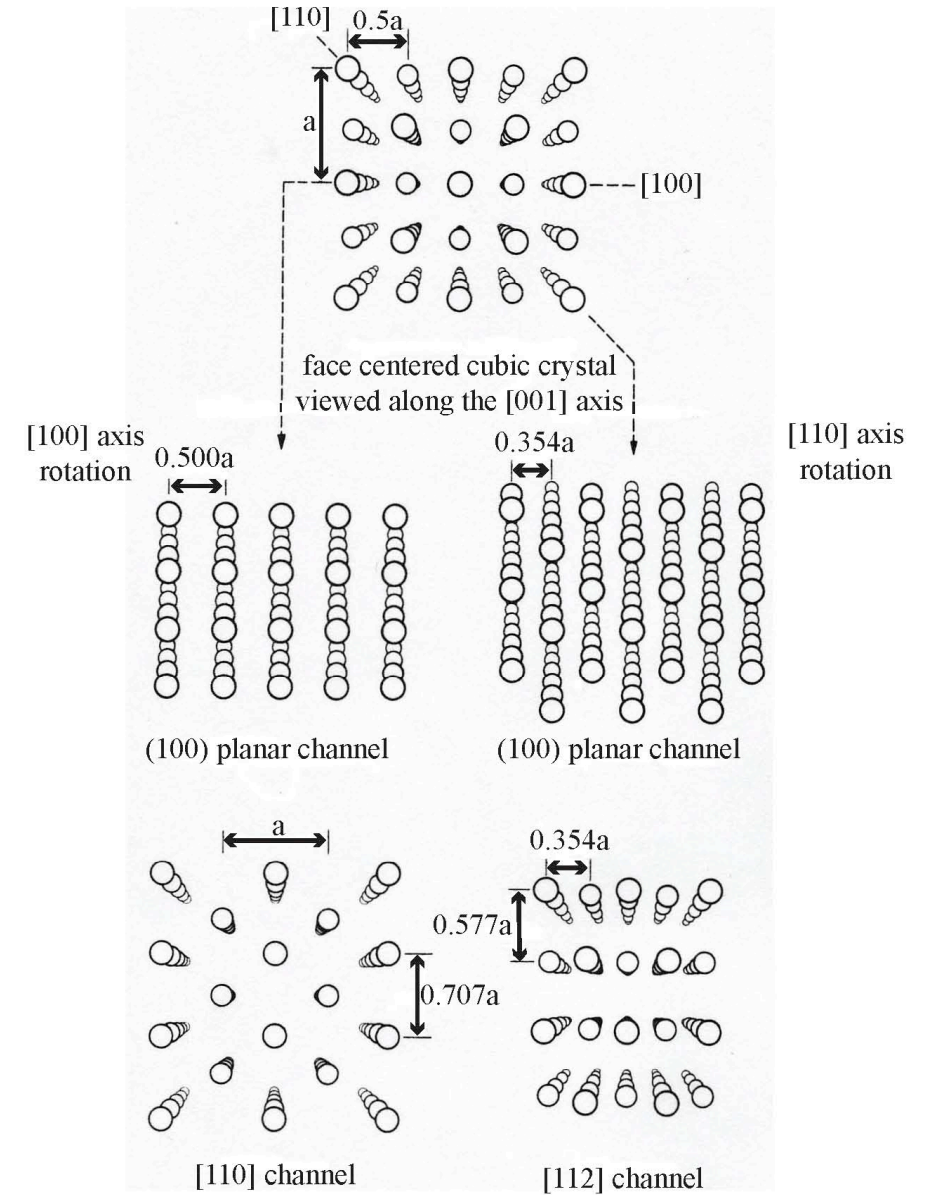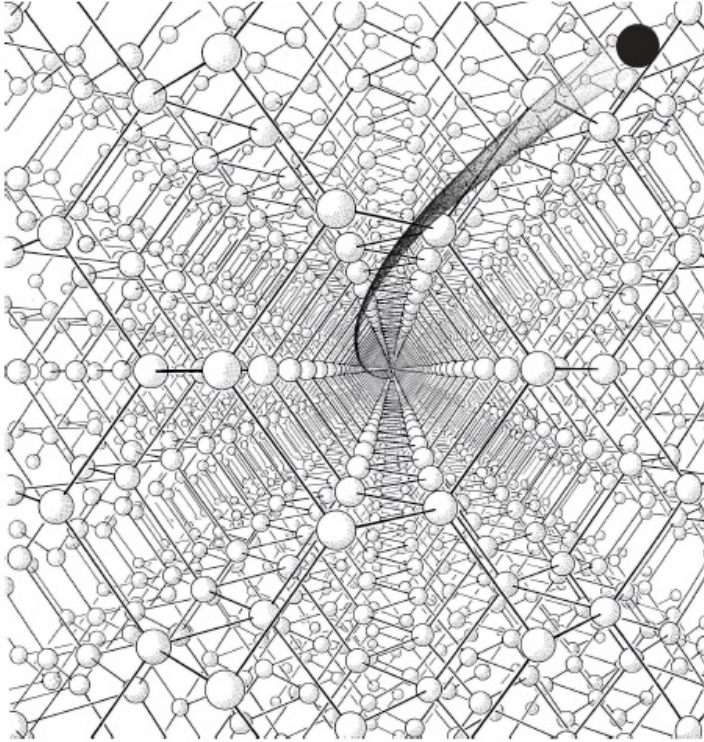Focusing   Channeling

Channeling

Down a primary zone axis

Down a random orienation
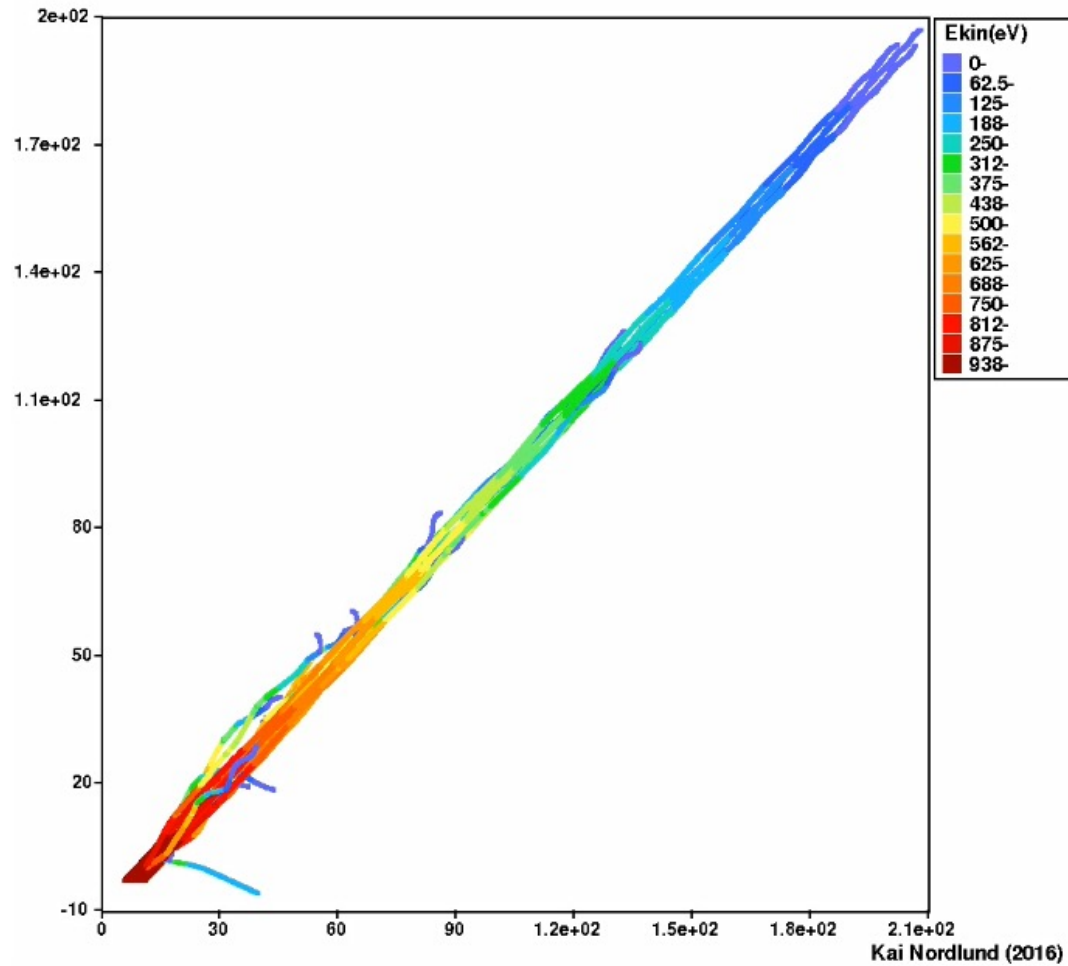
Images from Kai Nordlund

Channeling

[110]   0.5a

a

[100]

face centered cubic crystal
viewed along the [001] axis

[100] axis
rotation   0.500a

0.354a   [110] axis
rotation

(100) planar channel   (100) planar channel

a

0.354a

0.577a

0.707a

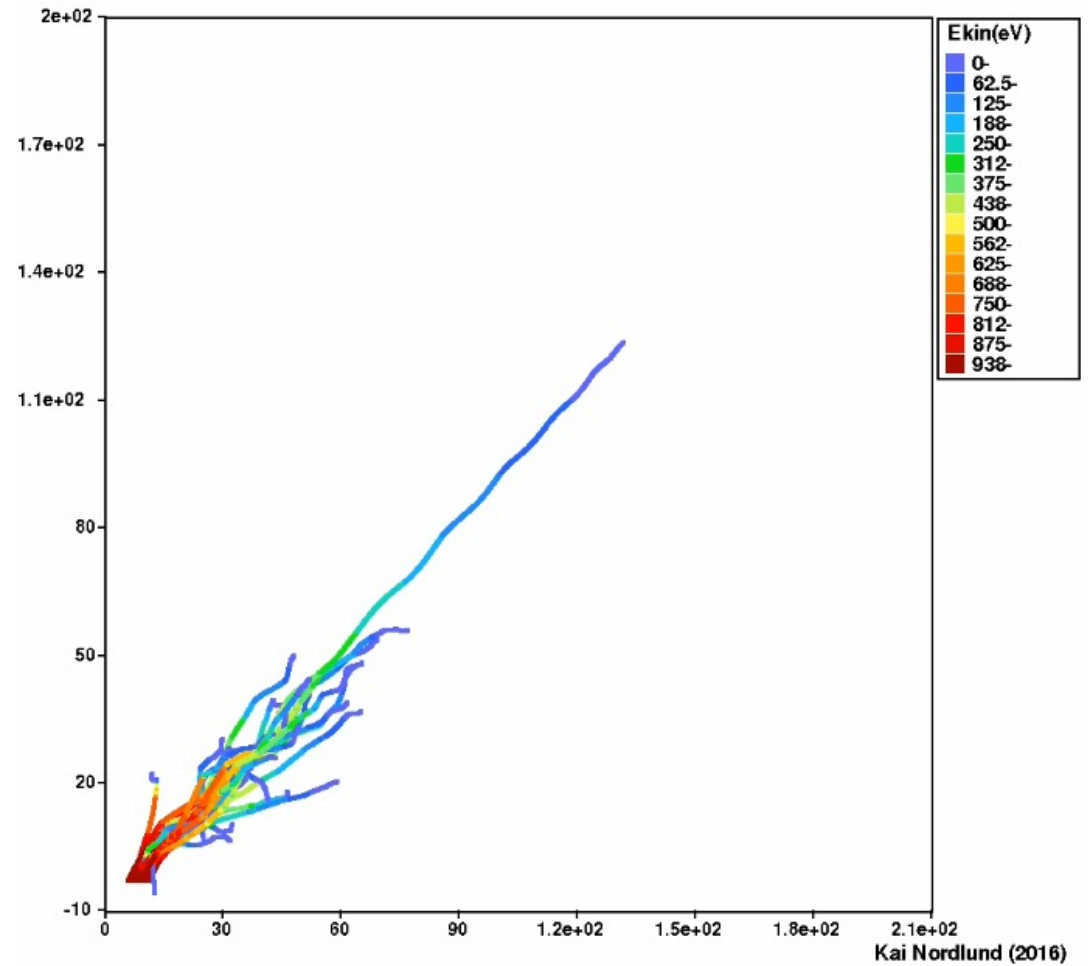[110] channel   [112] channel

Channeling illustration

30 individual 1 keV Si in Si ion trajectories, theta=45, phi=0

30 individual 1 keV Si in Si ion trajectories, theta=30, phi=0

Kai Nordlund (2016)

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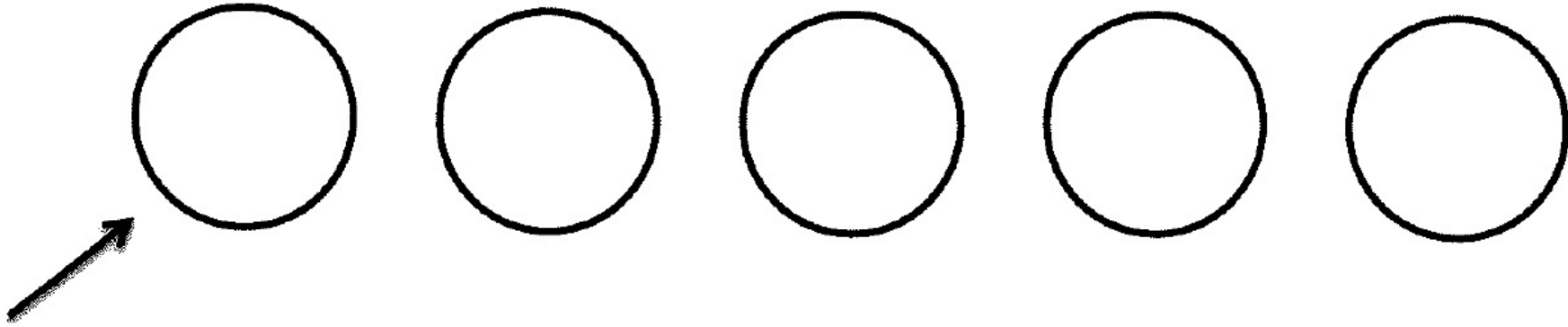RADIOLOGICAL SCIENCES
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Channeling

- Channeling is a high energy process

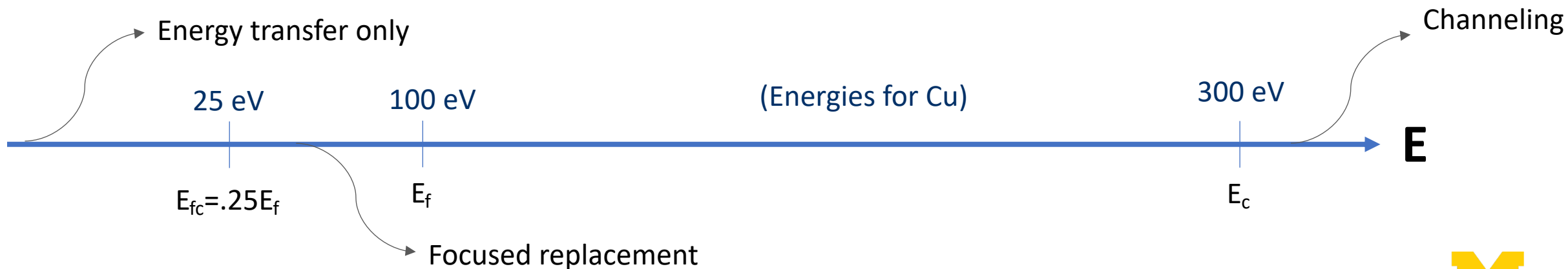# Practical Applications of Channeling
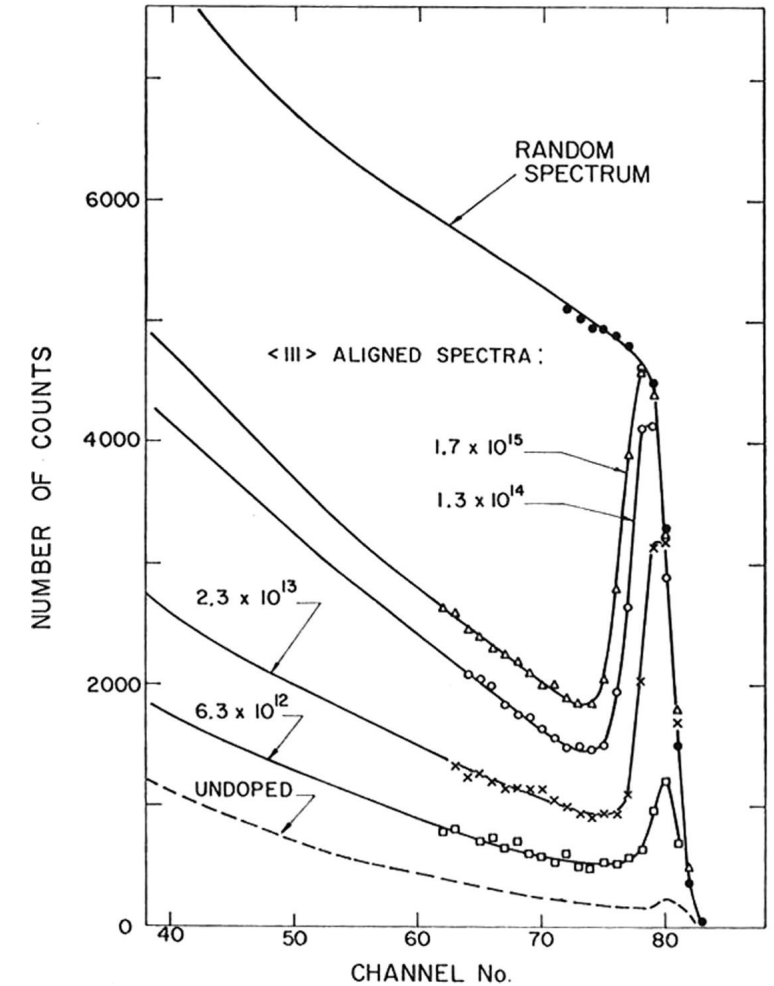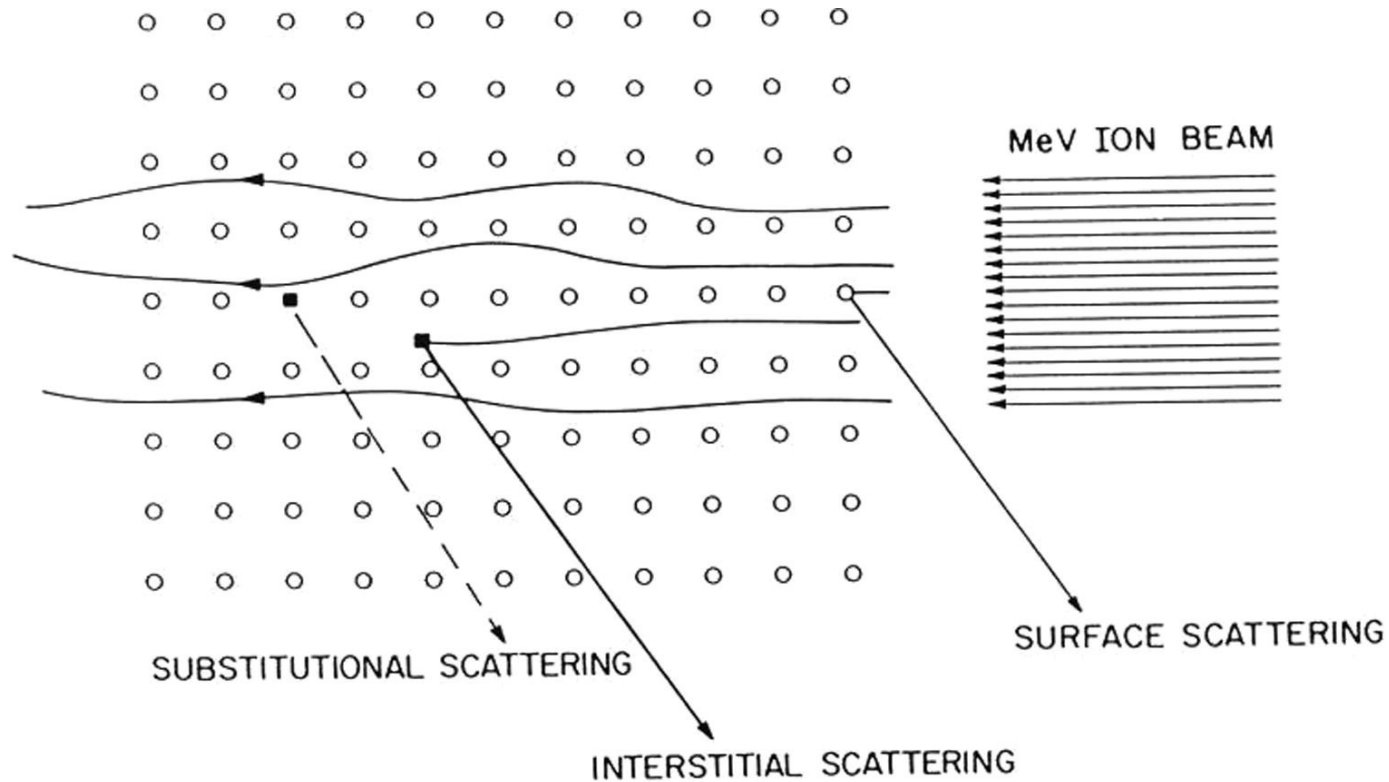
Focusing

- Close-packed energy transfer
- Simplest formalism assumes hard sphere collisions

Energy transfer only

Channeling

25 eV   100 eV   (Energies for Cu)   300 eV

$E_{fc}=.25E_f$ E_f E_c **E**

Focused replacement

Coming back to determining v(T)

Assumption	Correction to $v(T)$	Equation in text
#3 – loss of E_d	$0.56\left(1+\dfrac{T}{2E_d}\right)$	(2.31)
#4 – electronic energy loss cut-off	$\xi(T)\left(\dfrac{T}{2E_d}\right)$	(2.50)
#5 – realistic energy transfer cross-section	$C\dfrac{T}{2E_d},\ 0.52 \leq C \leq 1.22$	(2.33), (2.39)
#6 – crystallinity	$\dfrac{1-P}{1-2P}\left(\dfrac{T}{2E_d}\right)^{(1-2P)}-\dfrac{P}{1-2P}$	(2.104)
	$\sim\left(\dfrac{T}{2E_d}\right)^{(1-2P)}$	(2.105)

NRT Model

- NRT:

Accounts for Frenkel pair defect efficiency

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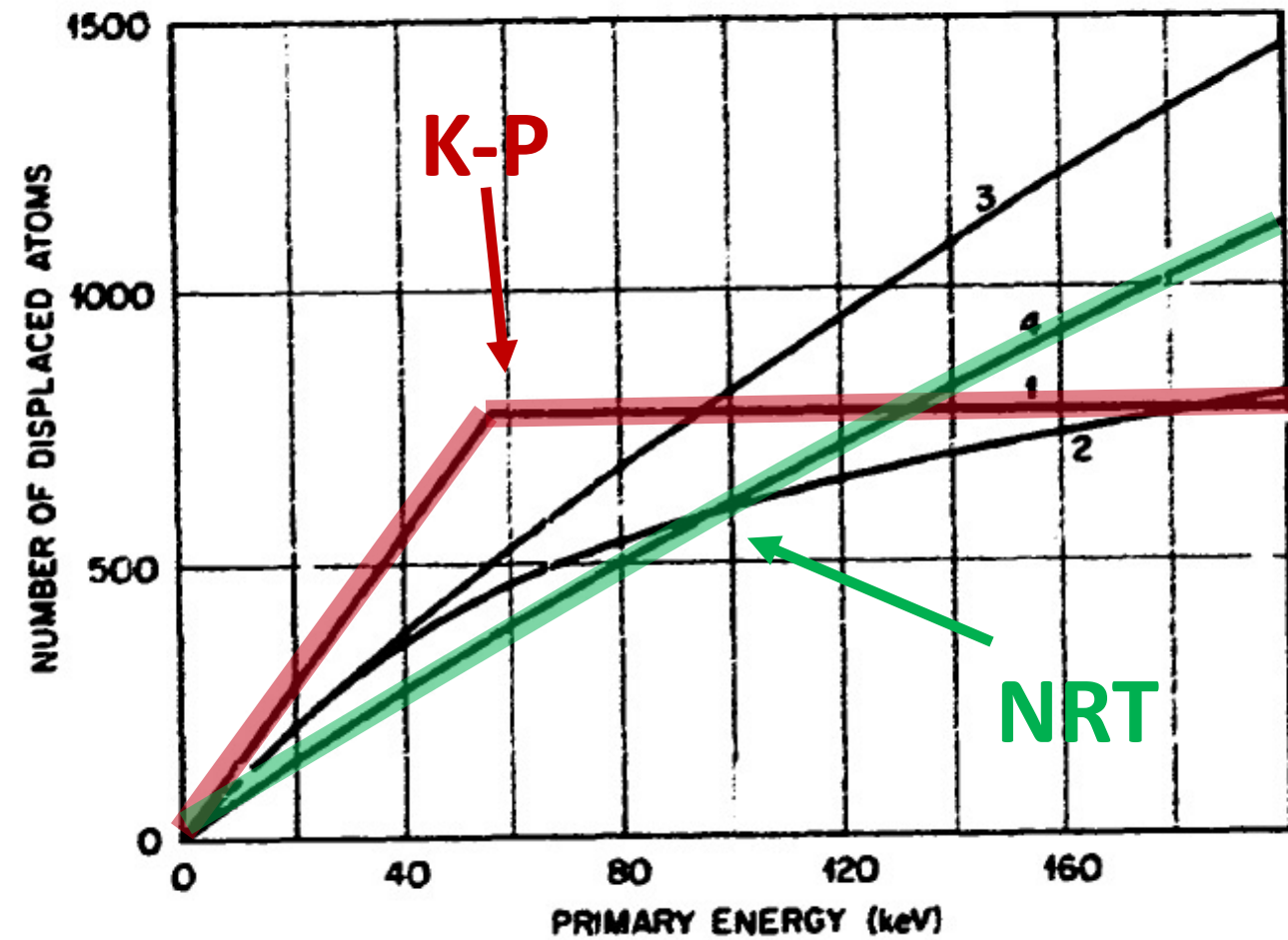

Fig. 2. Comparison of number of displaced atoms generated in bcc iron by a primary knock-on atom. Calculated results correspond to: (1) Kinchin–Pease model with $E_d = 40$ eV and $E_1 = 56$ keV; (2) the half-Nelson formula [4]; (3) earlier computer calculations of Norgett [18], using Torrens–Robinson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

Arc-dpa model

- Over the past 30 years it has become clear that the NRT method for determining dpa in metals is not correct

    - This is due to recombination, which we'll discuss in a few lectures

- To correct the NRT model, the "athermal-recombination corrected dpa", arc-dpa equation was proposed:

$$N_{d,arcdpa}(T) = \begin{bmatrix} 0 & \text{when} & T < E_d \\ 1 & \text{when} & E_d < T < 2E_d \\ \dfrac{0.8\,T}{2E_d}\xi(T) & \text{when} & 2E_d < T < \infty \end{bmatrix}$$

$$\xi(T) = \frac{1 - c_{arcdpa}}{(2E_d/0.8)^{b_{arcdpa}}}T^{b_{arcdpa}} + c_{arcdpa}$$

Questions?