Modifications to K-P Displacement Model & Stopping Powers

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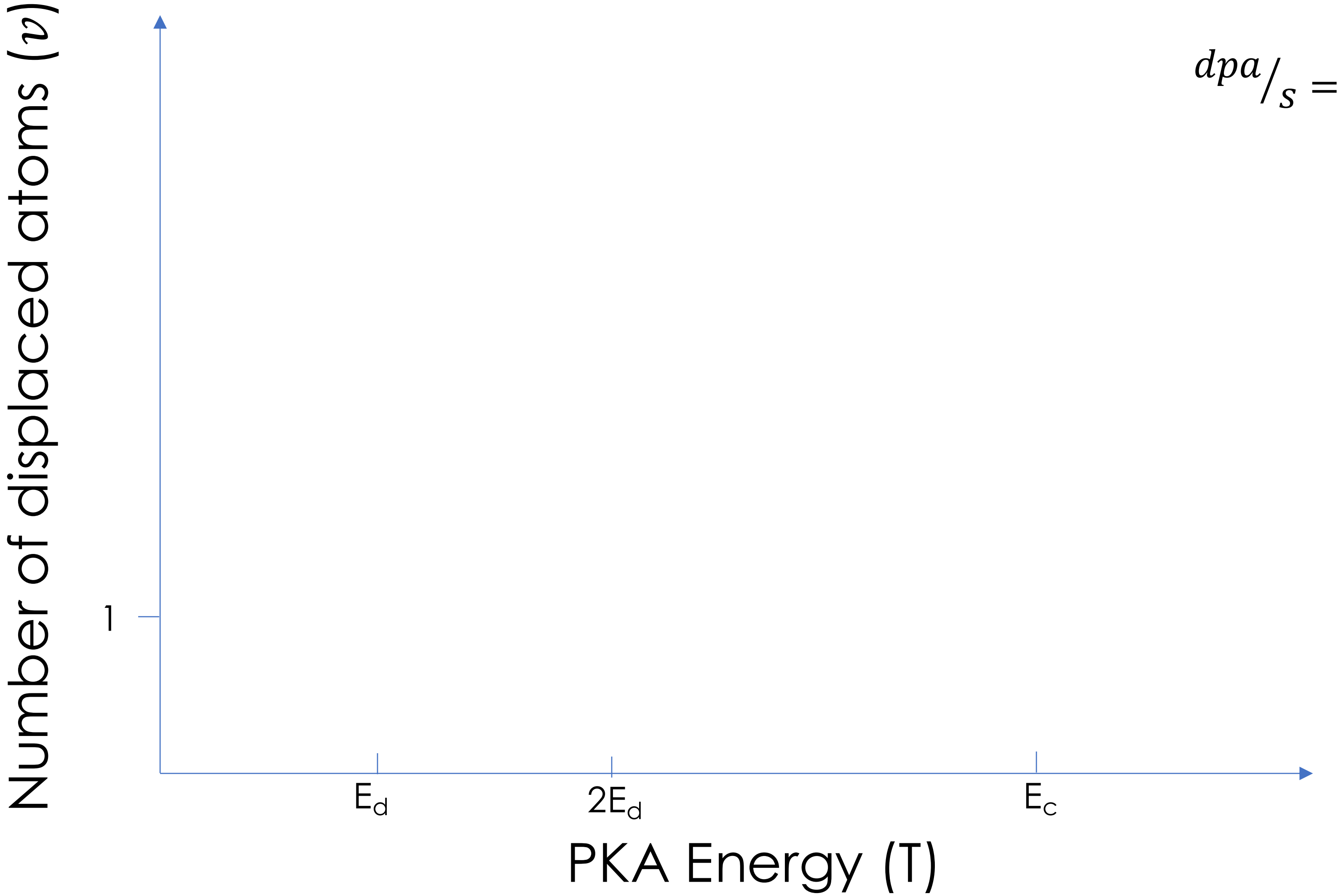
Summary of Topics Covered



$$dpa/_{s} = N \int_{\check{E}}^{\hat{E}} \Phi(E_i) \int_{\check{T}}^{\hat{T}} \sigma(E_i, T)\, \nu(T)\, dT\, dE_i$$

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Brain storming

- Why would the K-P model not be correct? (but reasonable)

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

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A simple picture of slowing down

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

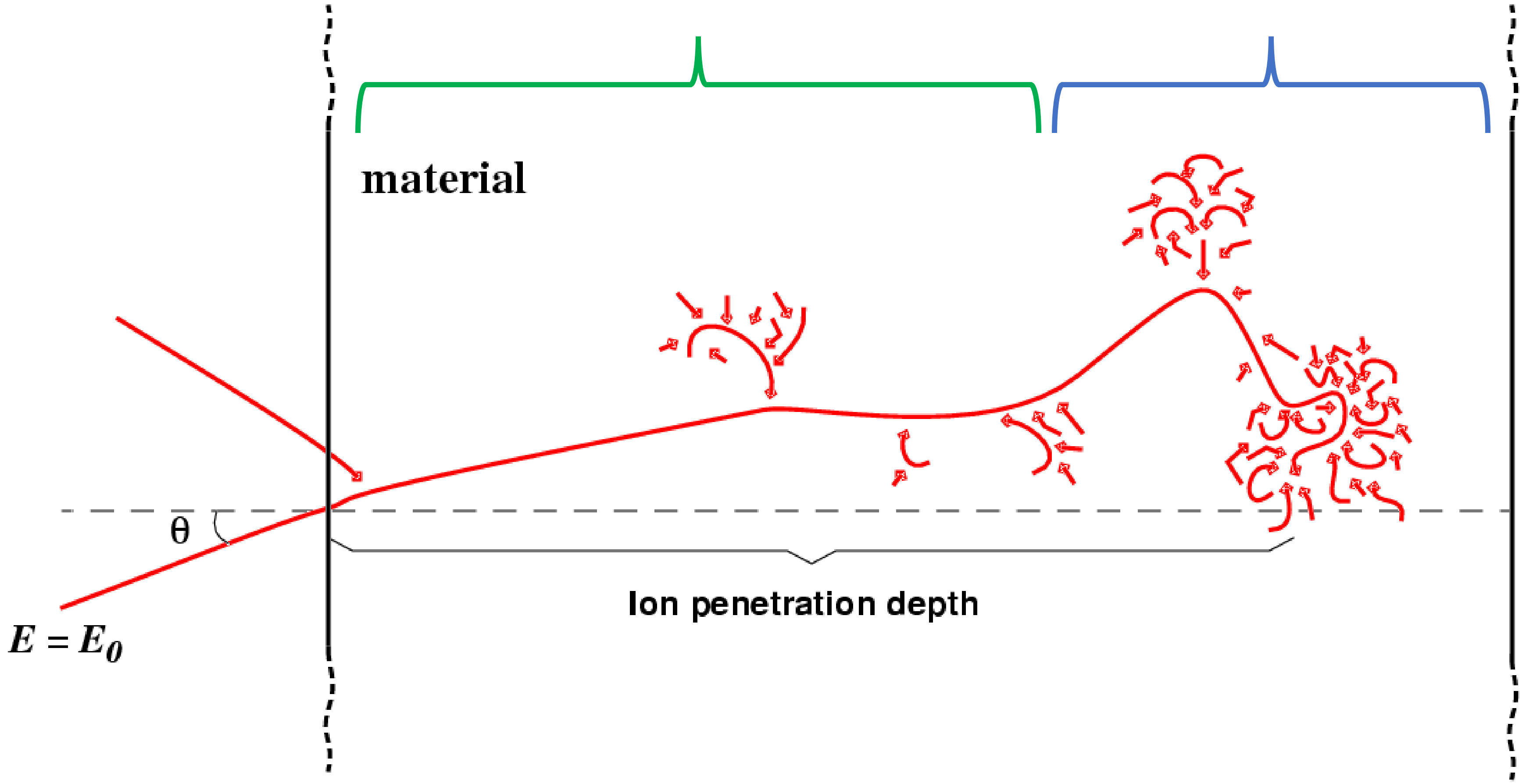
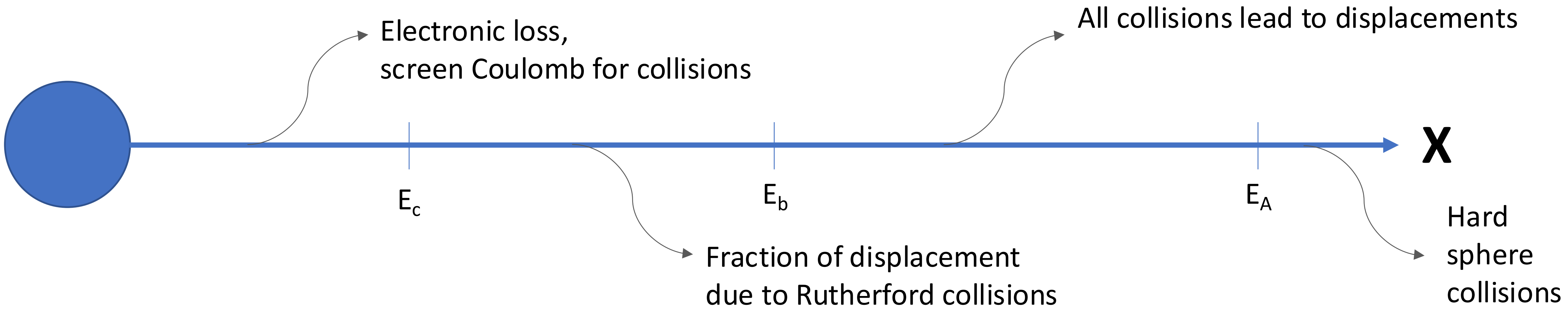


Image: Kai Nordlud

Regimes of energy loss of a PKA



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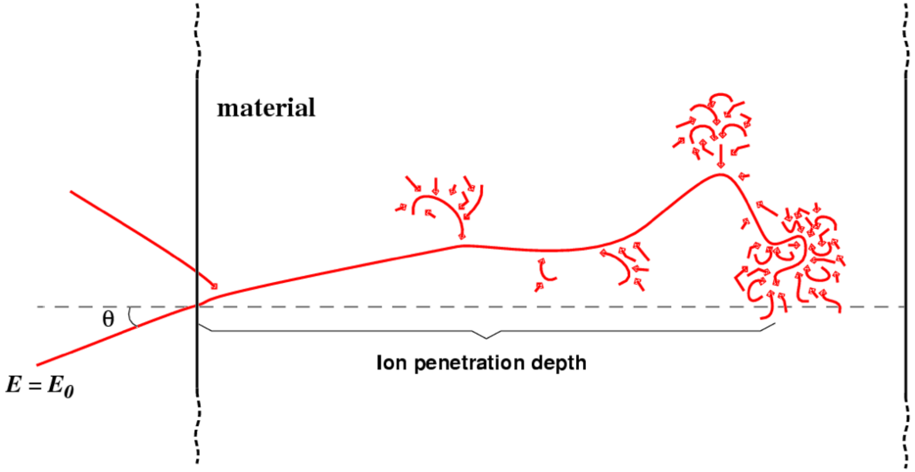
The concept of stopping power

- Since the electronic collisions only slow down the ion, 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**



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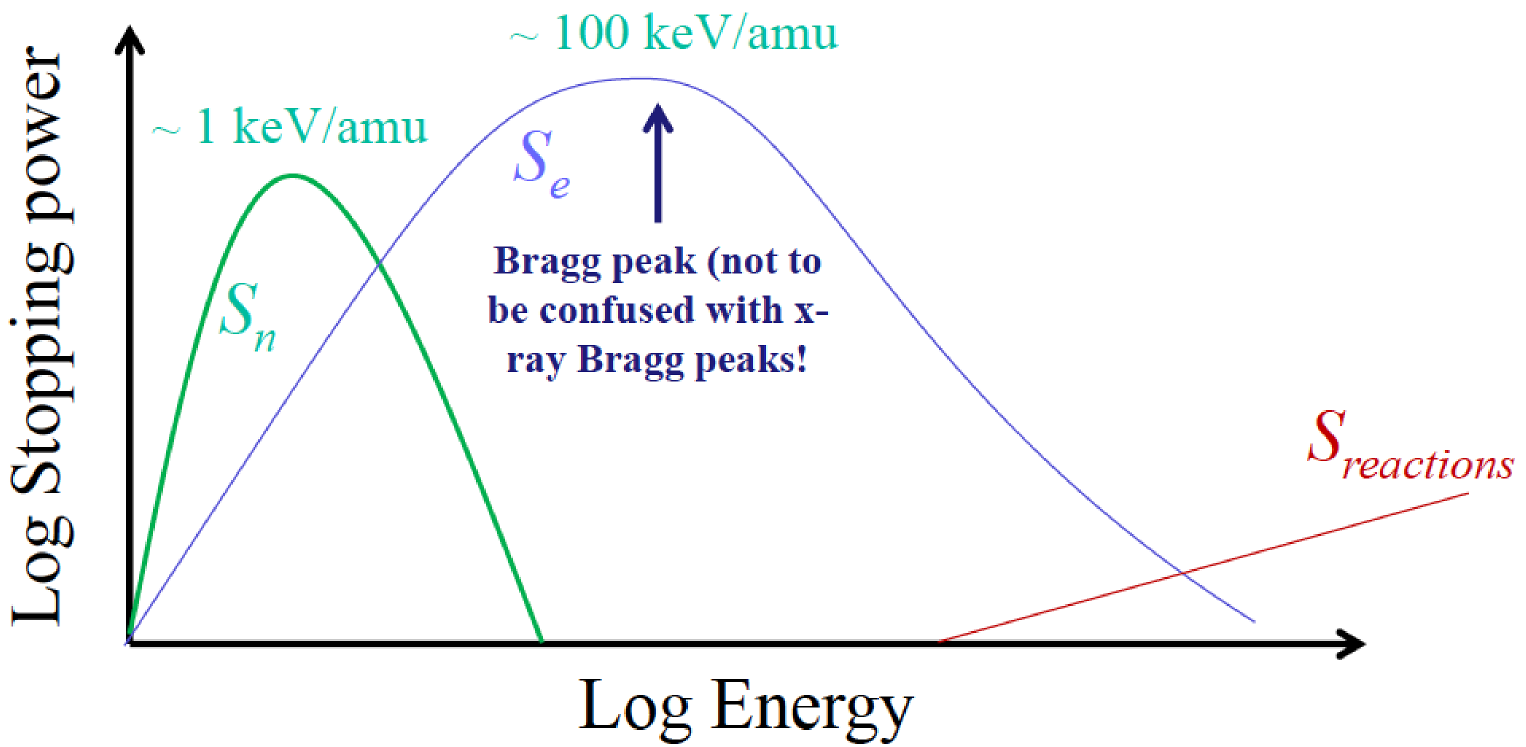
Stopping power

- The total stopping power can be written as

- Schematically, the energy dependence of these is then:



Slide: Kai Nordlud

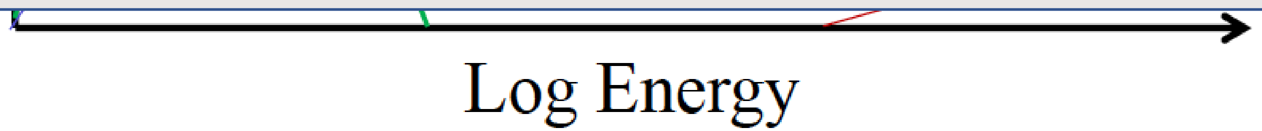
Stopping power

- 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**



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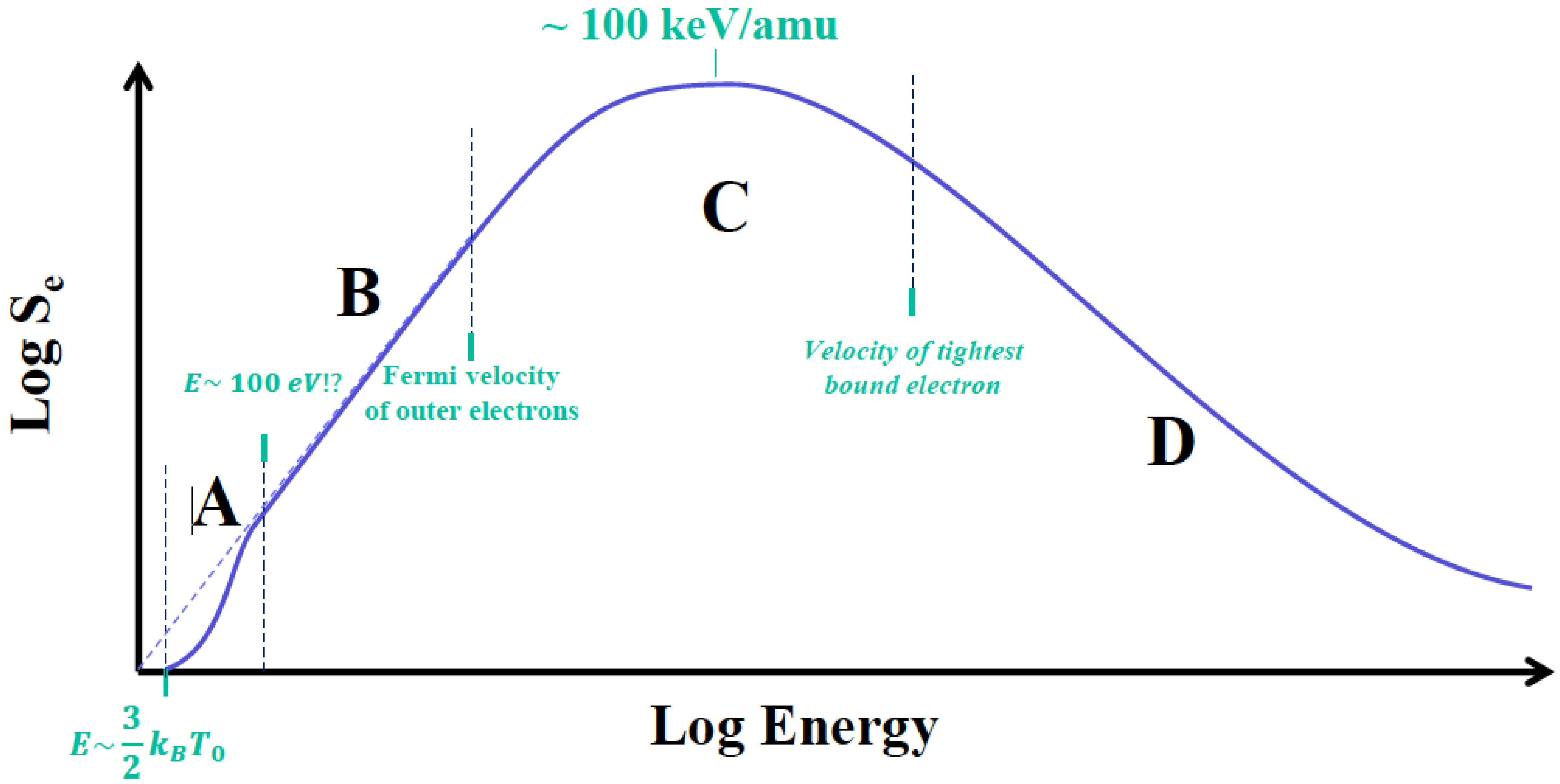
Regimes of electronic stopping power

- Electronic stopping can be segregated into four primary regimes:



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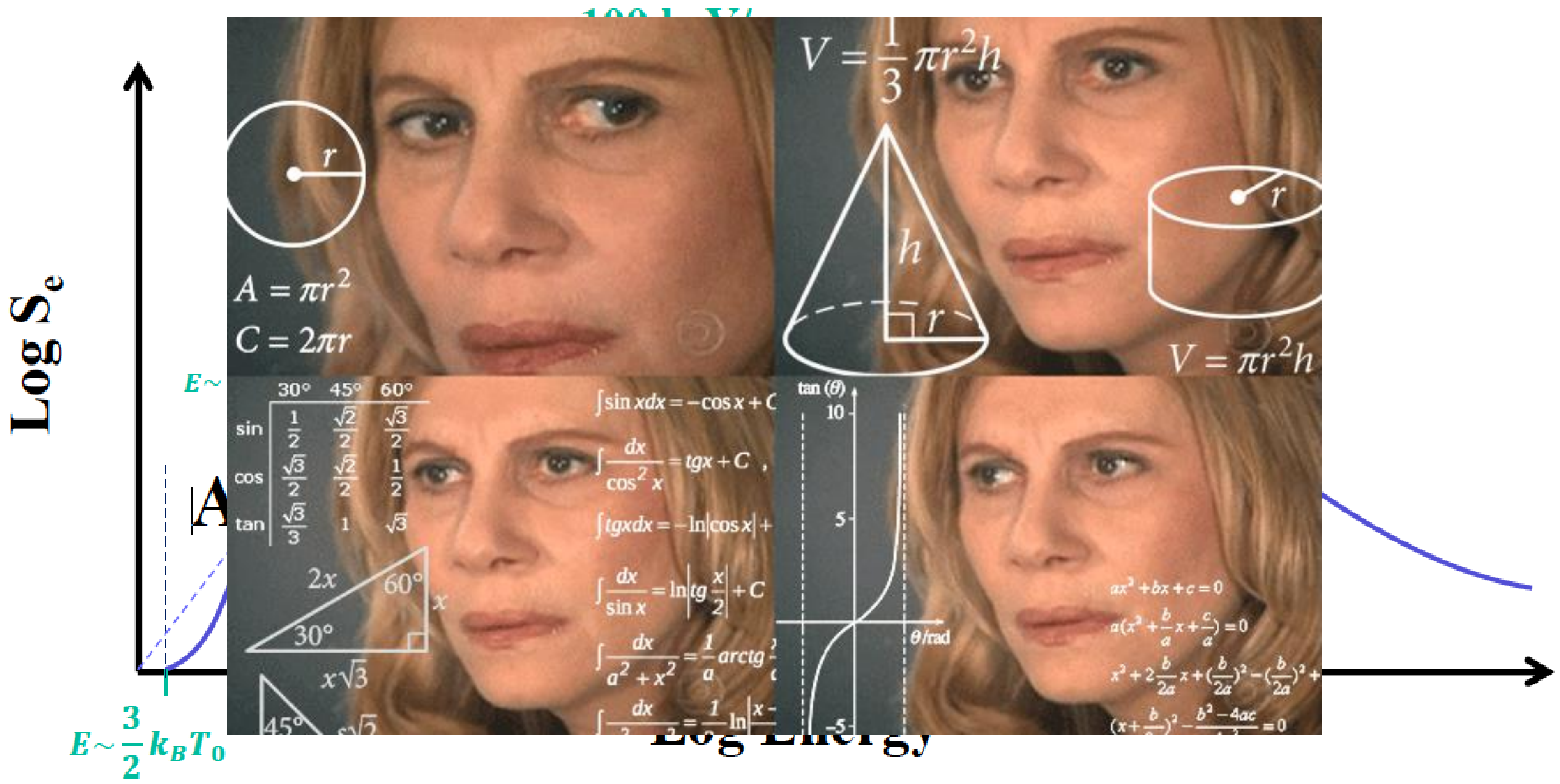

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Stopping powers

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

$$\left(-\frac{dE}{dx}\right)_{total} = NS_n + NS_e$$

- Nuclear:

$$\left(-\frac{dE}{dx}\right)_n = \frac{N\pi Z_1 Z_2 \varepsilon^4}{E_i}\frac{M_1}{M_2} ln\left(\frac{\gamma E_i}{\frac{\varepsilon^2 \gamma E_a^2}{4E_i}}\right)$$

- Electronic:

$$\left(-\frac{\mathrm{d}E}{\mathrm{d}x}\right)_{\mathrm{e}} = \frac{N2\pi Z_1^2 Z_2 \varepsilon^4}{E_{\mathrm{i}}}\frac{M}{m_{\mathrm{e}}}\ln\left(\frac{\gamma_{\mathrm{e}}E_{\mathrm{i}}}{\bar{I}}\right) = \frac{2\pi N Z_1^2 M \varepsilon^4}{m_{\mathrm{e}}E_{\mathrm{i}}}B \qquad B = Z_2 \ln\left(\frac{\gamma_{\mathrm{e}}E_{\mathrm{i}}}{\bar{I}}\right)$$

Relative Stopping Powers

- Compare S_e/S_n:

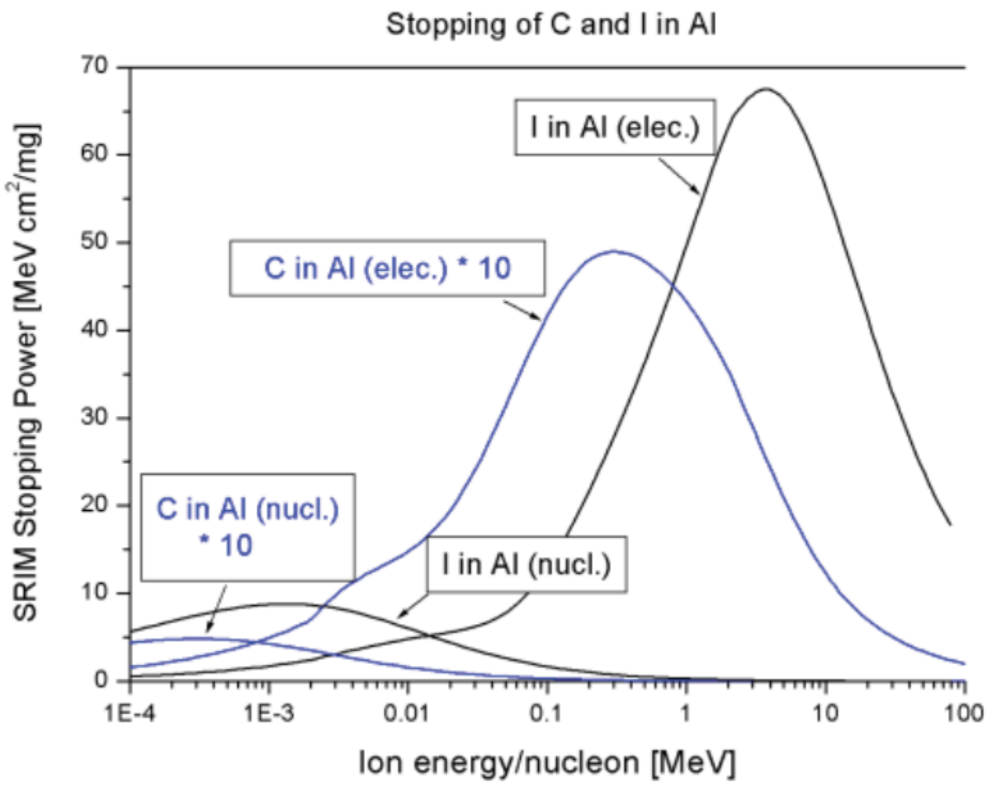

FIGURE 2. Electronic and nuclear mass stopping power for carbon and iodine ions in aluminum, calculated using SRIM.

- Electronic stopping power dominates for high energy ions

https://doi.org/10.1063/1.4802339

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Stopping powers

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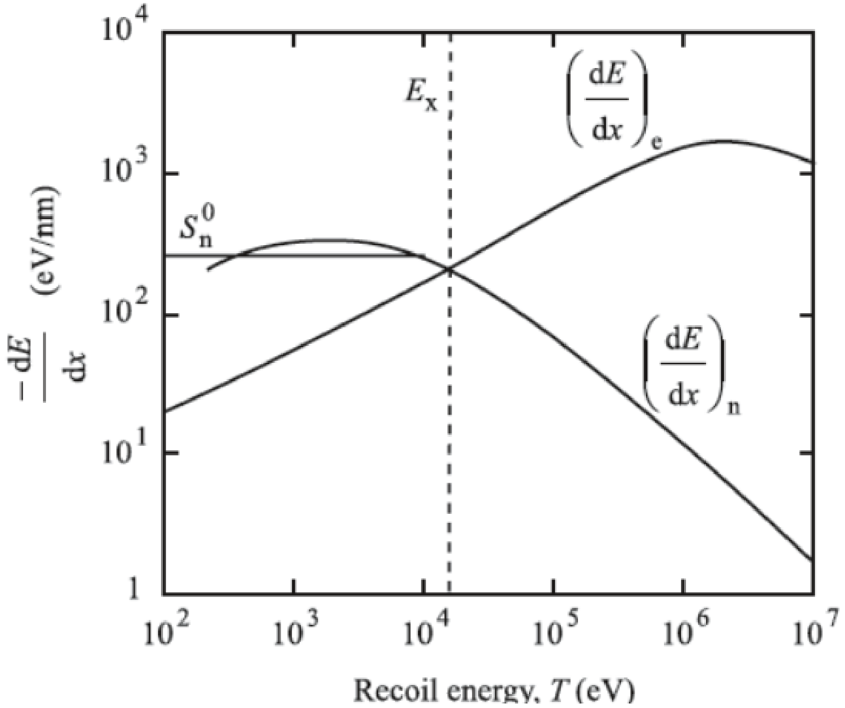
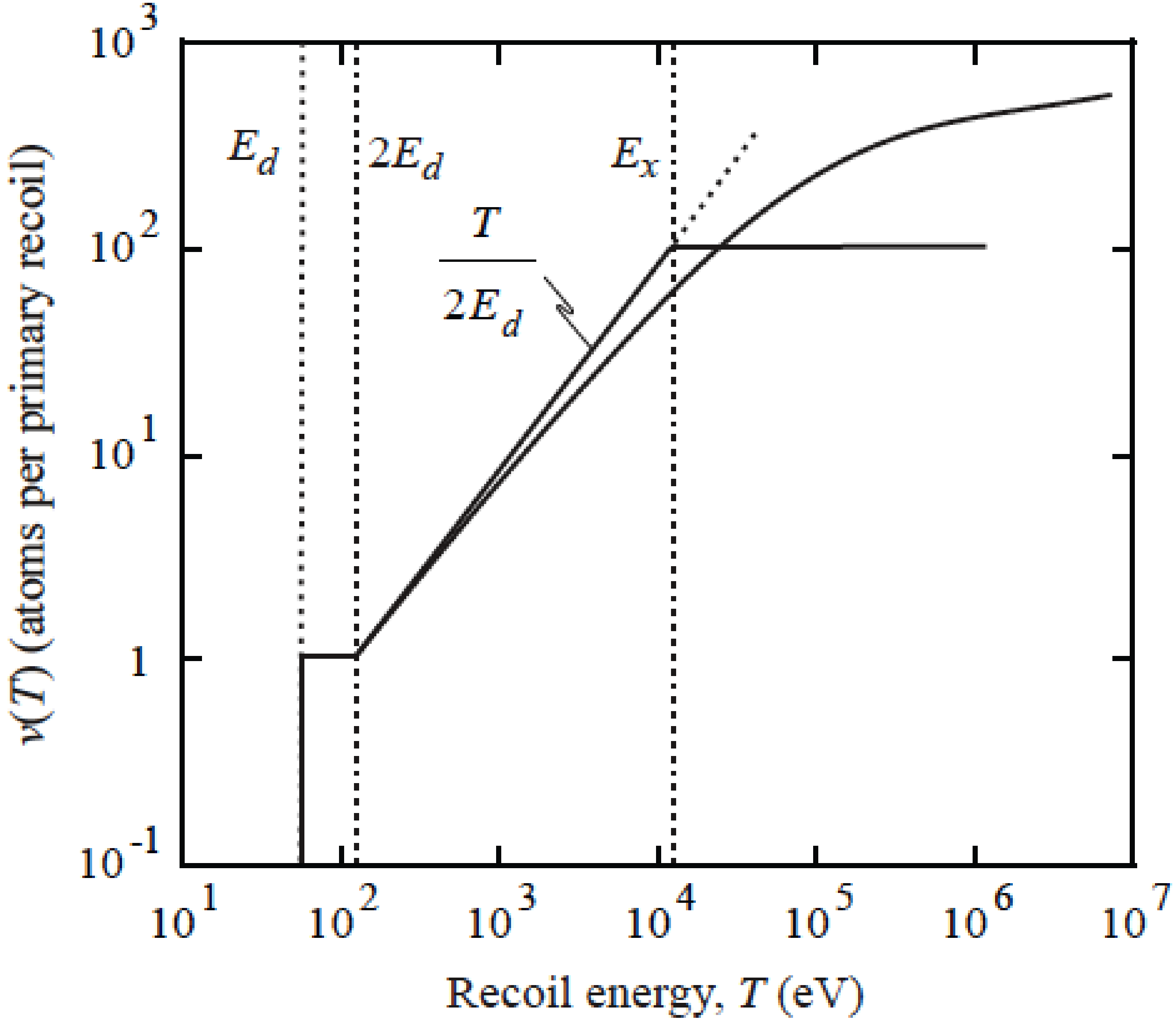
Table 1.7 Summary of energy loss rates for various types of interactions

Type of interaction	Nuclear energy loss rate $\left(-\frac{dE}{dx}\right)_n$		Electronic energy loss rate $\left(-\frac{dE}{dx}\right)_e$	
High E Coulomb	$\frac{4N\pi Z^4 a_0^2 E_R^2}{E_i}\ln\left(\frac{a^2c^2E_i^2}{4a_0^2E_R^2Z^4}\right)$	(1.134)	$N\pi\frac{Z_1^2Z_2\varepsilon^4}{E_i}\frac{M}{m_e}\ln\left(\frac{\gamma_e E_i}{\bar{I}}\right)$	(1.173)
Low E	General expression: $\frac{8.462\times10^{-15}NZ_1Z_2M_1S_n(\epsilon)}{(M_1+M_2)(Z_1^{0.23}+Z_2^{0.23})}$	(1.169)	$k'E_i^{1/2}$ $k'=3.83\frac{Z_1^{7/6}Z_2}{M_1^{1/2}\left(Z_1^{2/3}+Z_2^{2/3}\right)^{3/2}}$	(1.178) (1.179)
	Inverse square: $\frac{\pi^2}{4}a^2NE_a\gamma$	(1.159)	$kE_i^{1/2}$	(1.190)
	Thomas–Fermi screening: $K\frac{NZ_1Z_2}{Z^{1/3}}\frac{M_1}{M_1+M_2}$ where $Z^{1/3}=\left(Z_1^{2/3}+Z_2^{2/3}\right)^{1/2}$ and $K=\left(\frac{\pi}{e}\right)\varepsilon^2a_0=2.8\times10^{-15}\ \text{eV}\cdot\text{cm}^2$	(1.163)	$k=8\sigma_eN\left(\frac{m_e}{M_1}\right)^{1/2}$ valid for $0<E\ (keV)<37Z^{7/3}$	

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





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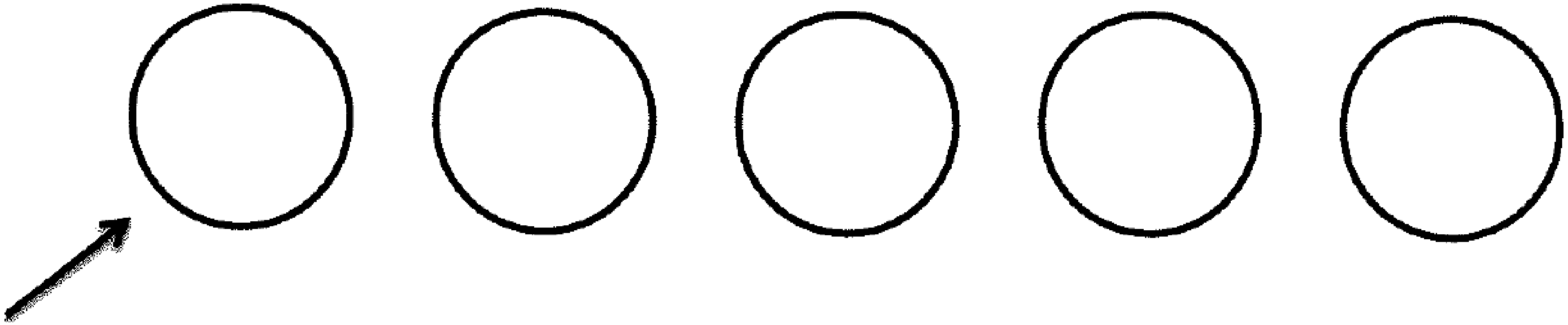
Modifications to K-P Model

2. Use of realistic cross sections

A simple thought experiment



To the document reader!

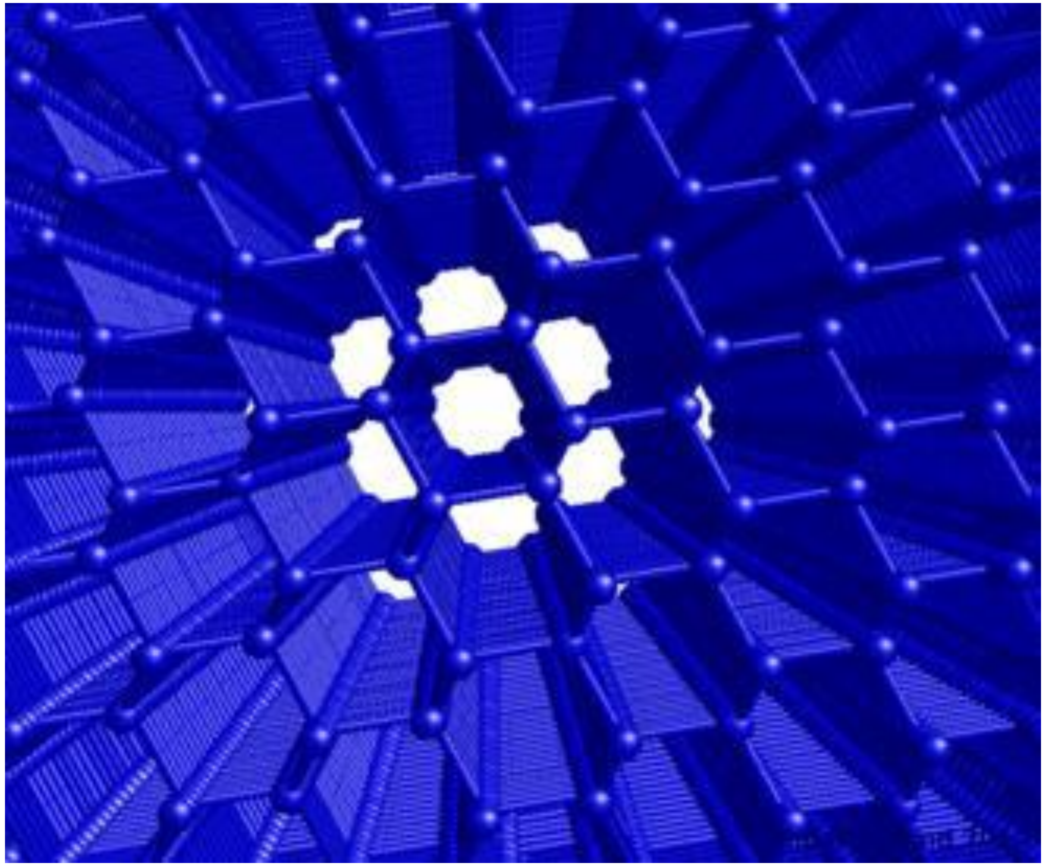
Modifications to K-P Model

3. Effect of crystallinity:

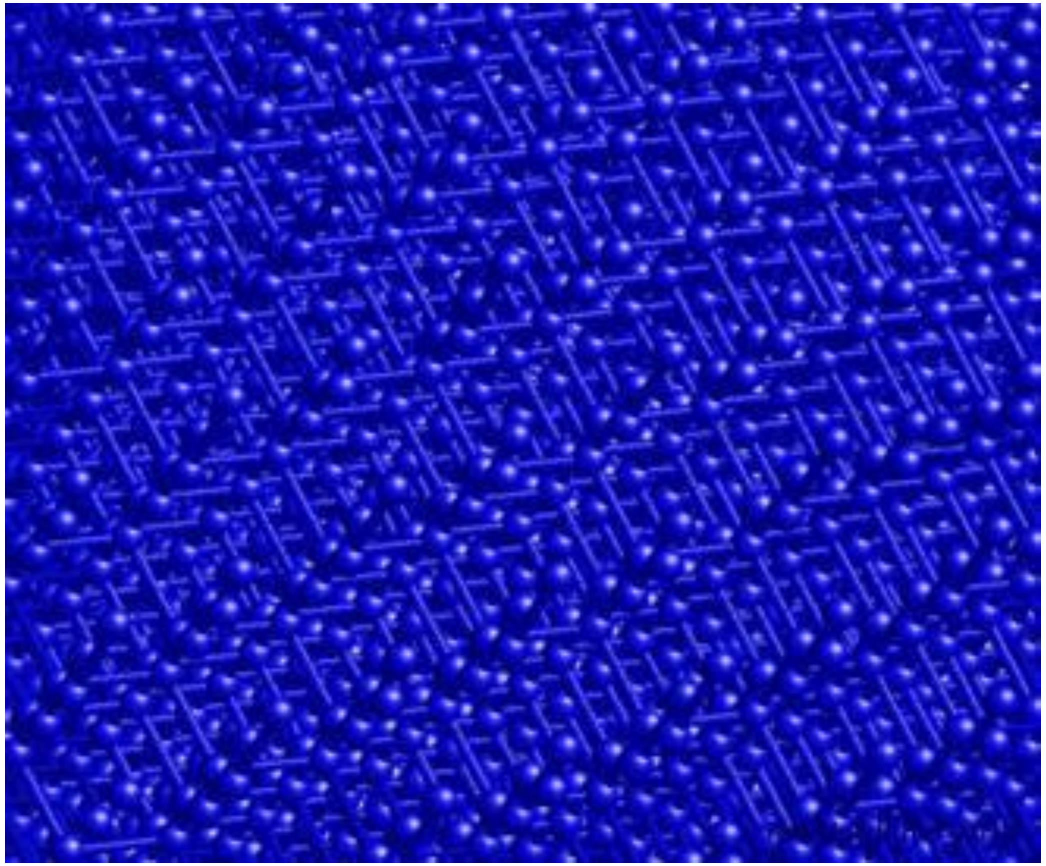
Focusing

Channeling

Channeling



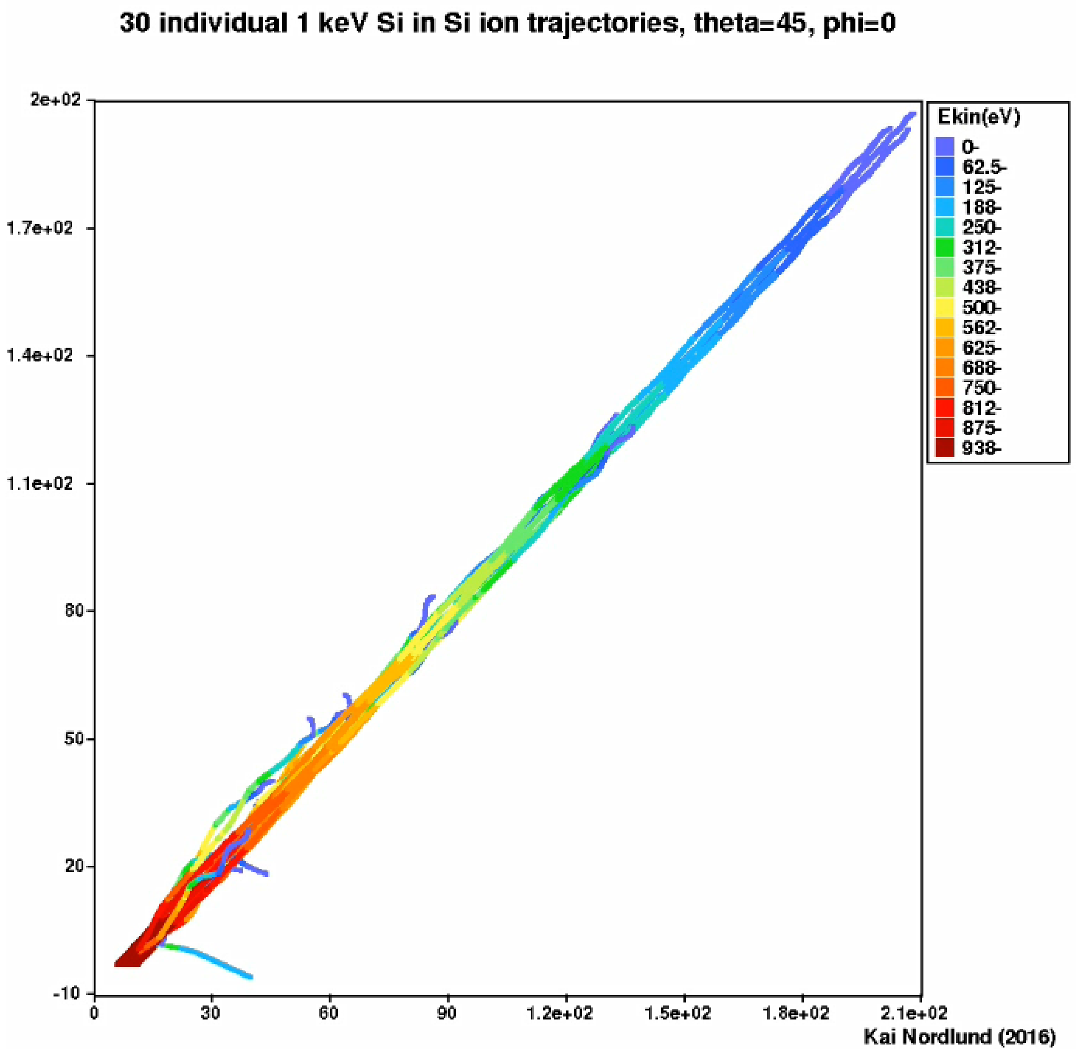
Down a primary zone axis

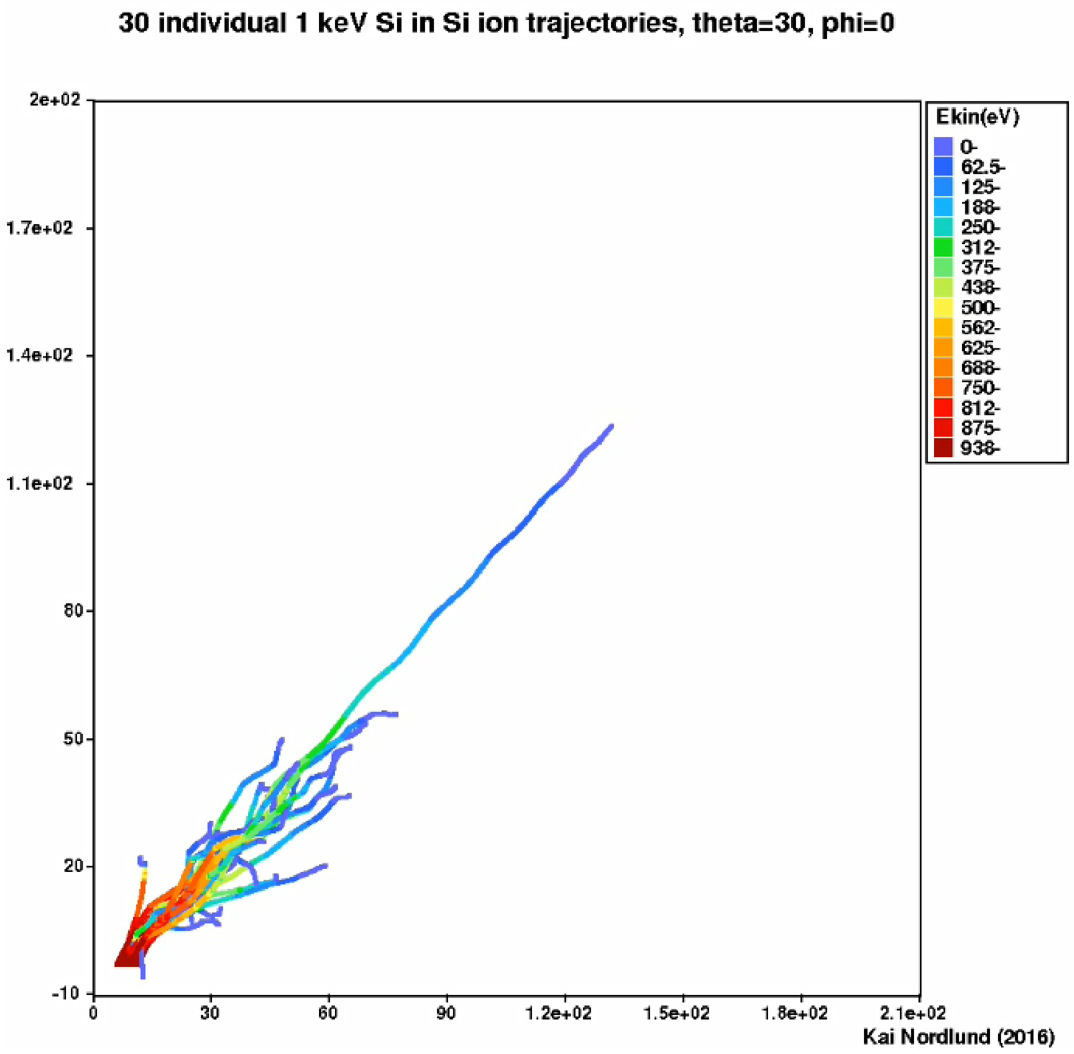


Down a random orienation

Images from Kai Nordlund

Channeling illustration





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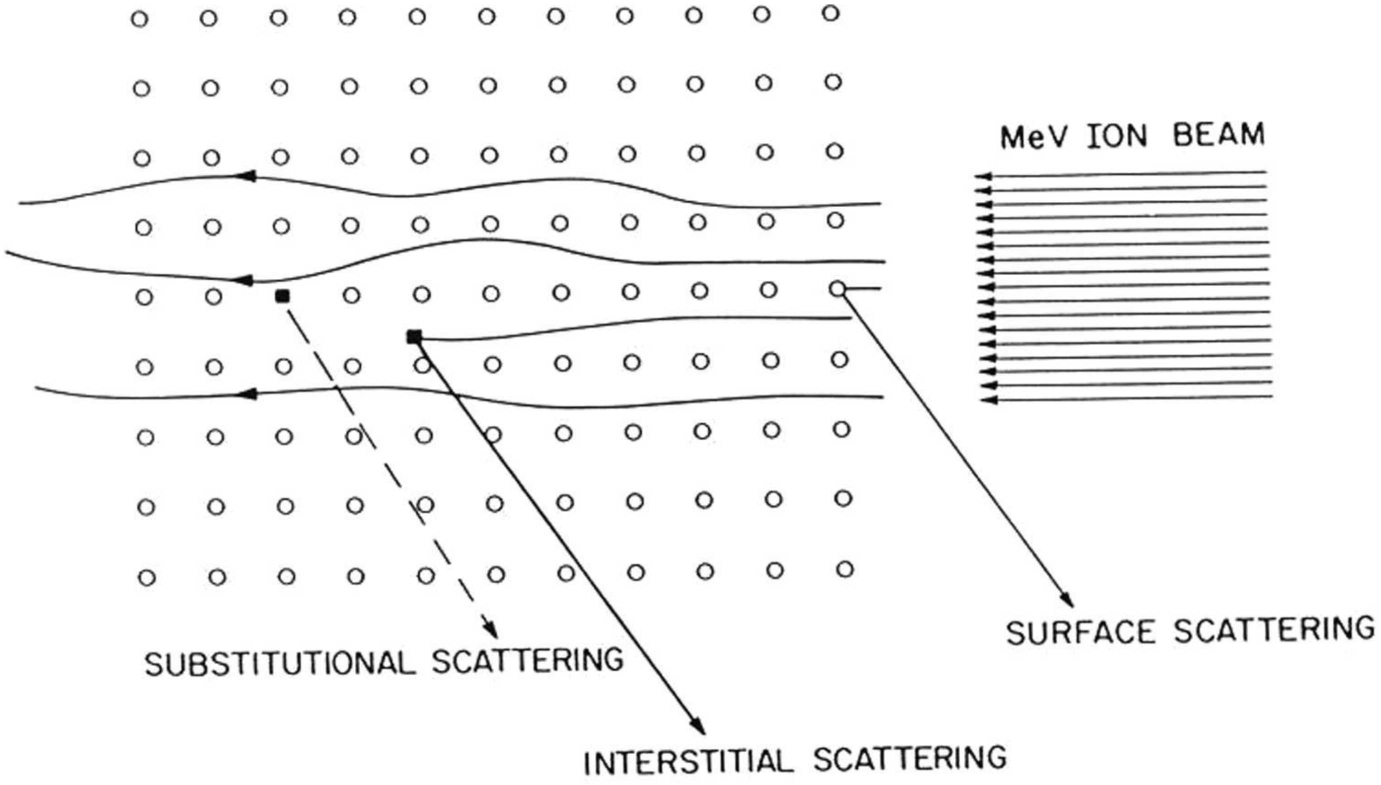
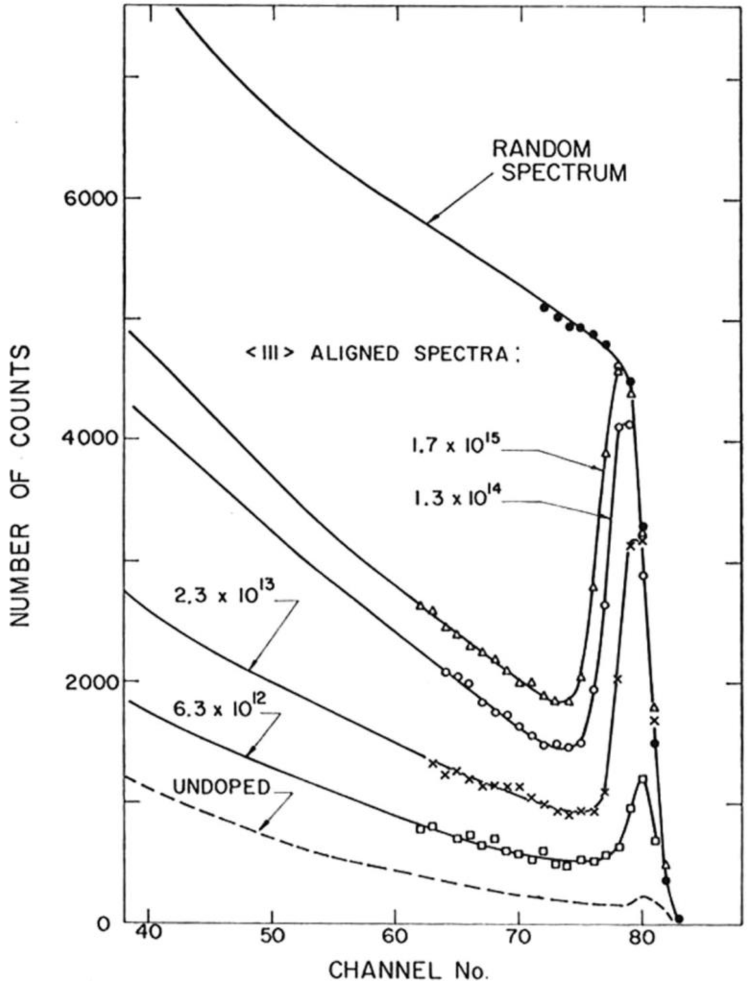
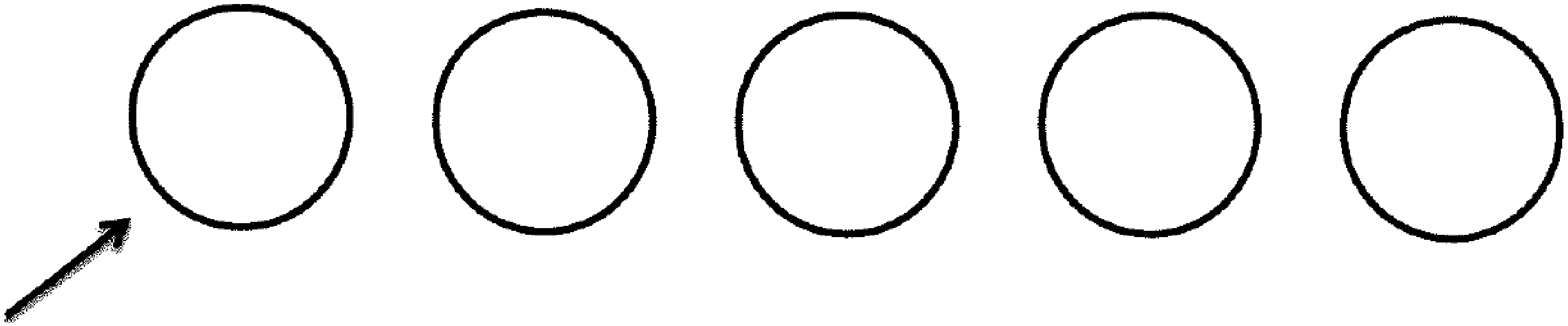
Practical Applications of Channeling



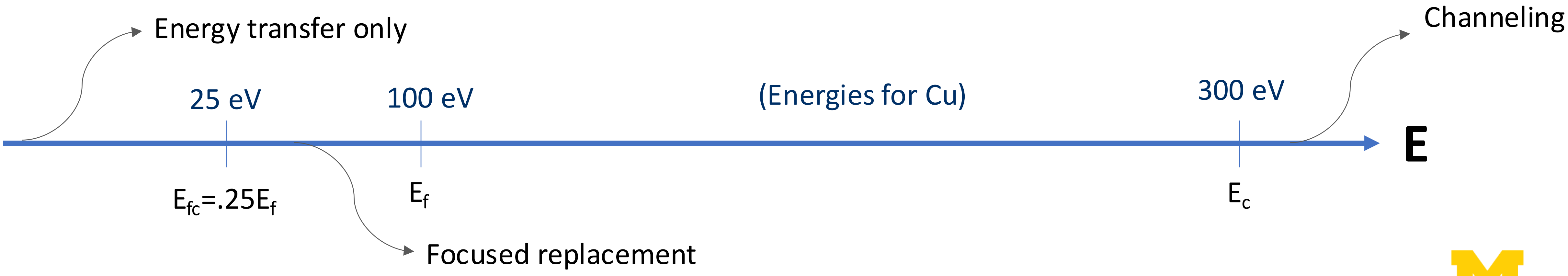


https://doi.org/10.1016/j.nimb.2015.11.035

Focusing



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



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Coming back to determining v(T)

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

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NRT Model

- NRT:

Accounts for Frenkel pair defect efficiency

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

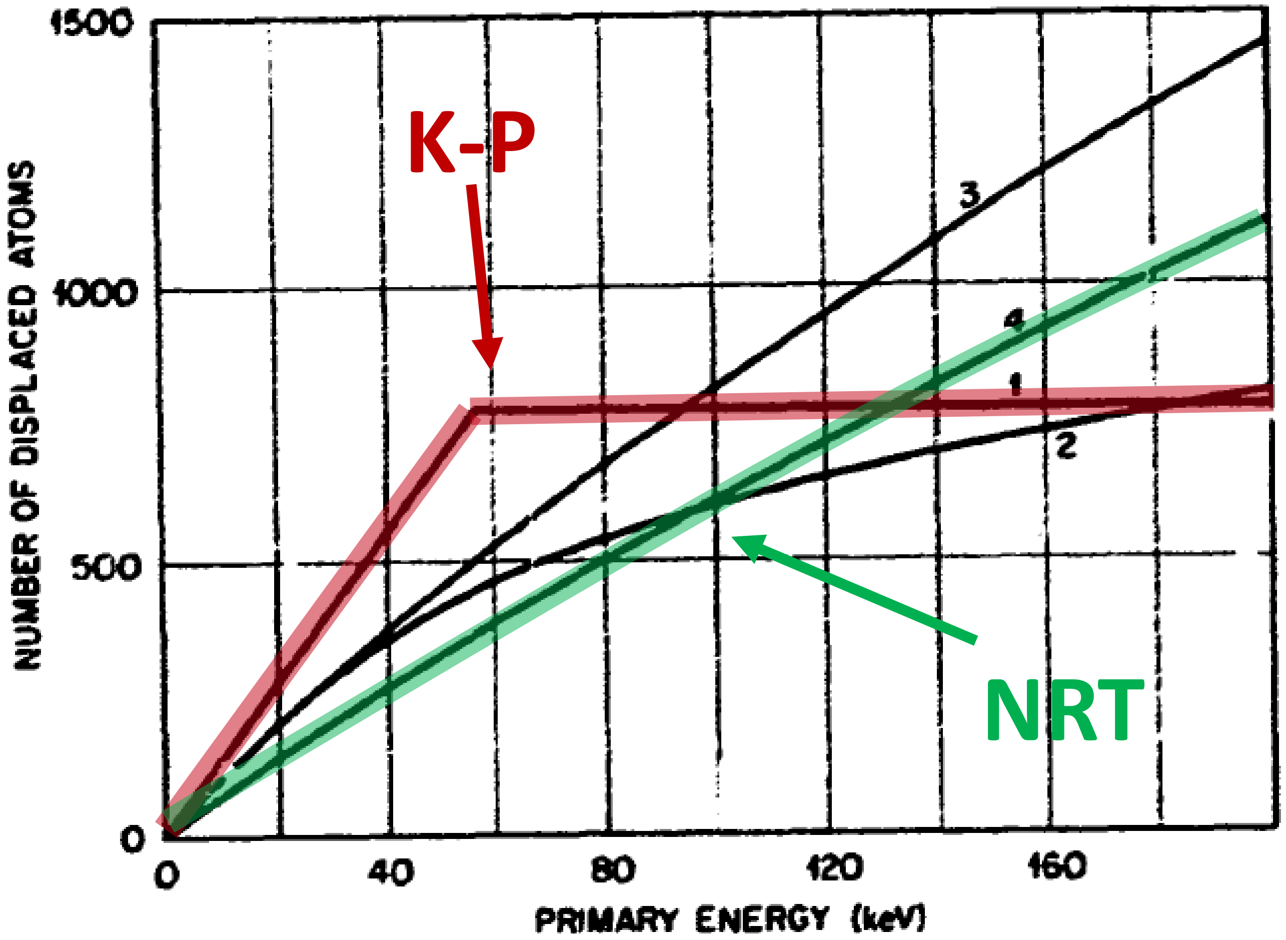

Fig. 2. Comparison of number of displaced atoms generated in bcc iron by a primary knock-on atom. Calculated results correspond to: (1) Kinchin–Pease model with E_d = 40 eV and E_1 = 56 keV; (2) the half-Nelson formula [4]; (3) earlier computer calculations of Norgett [18], using Torrens–Robinson computer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

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

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

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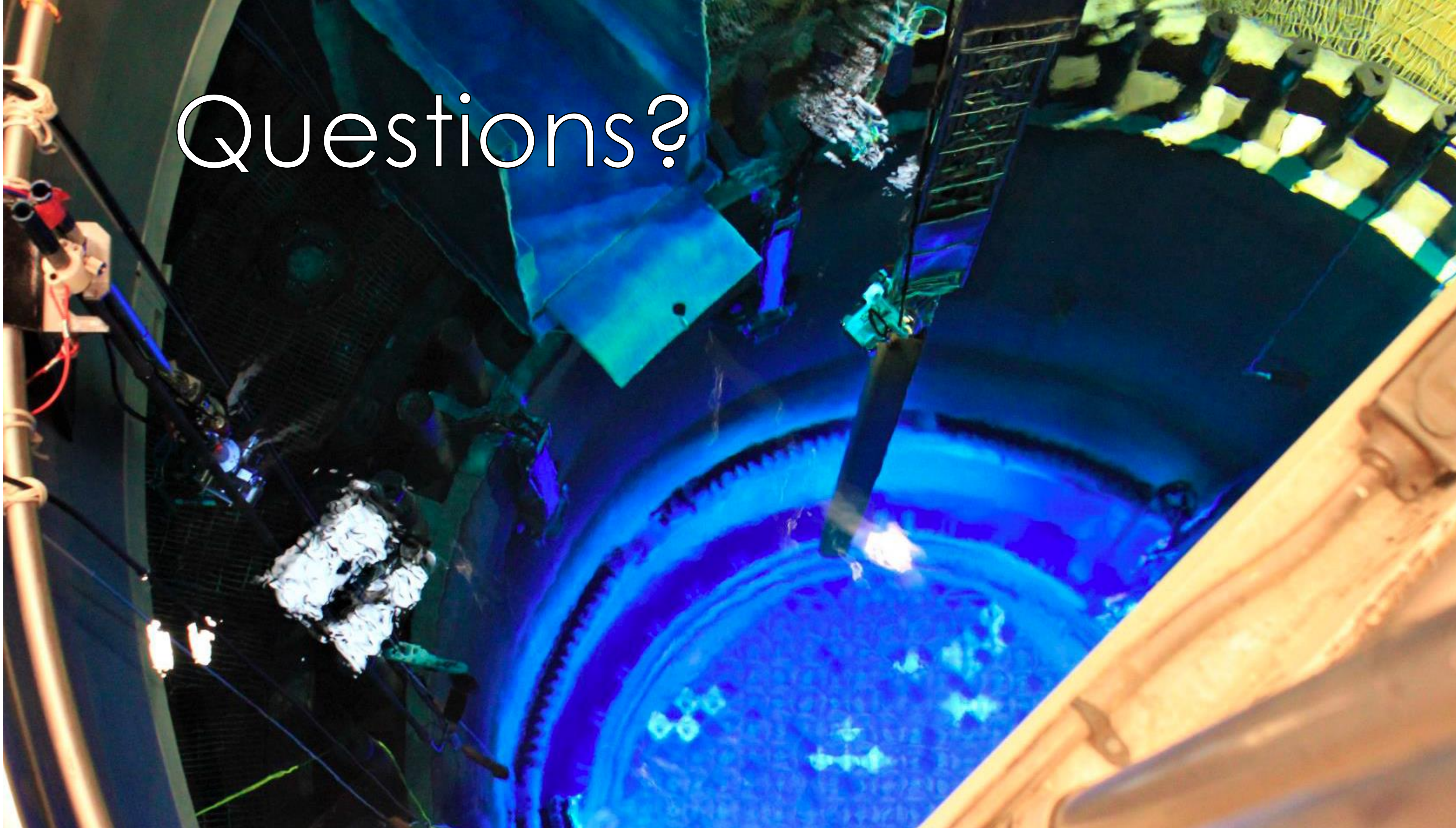
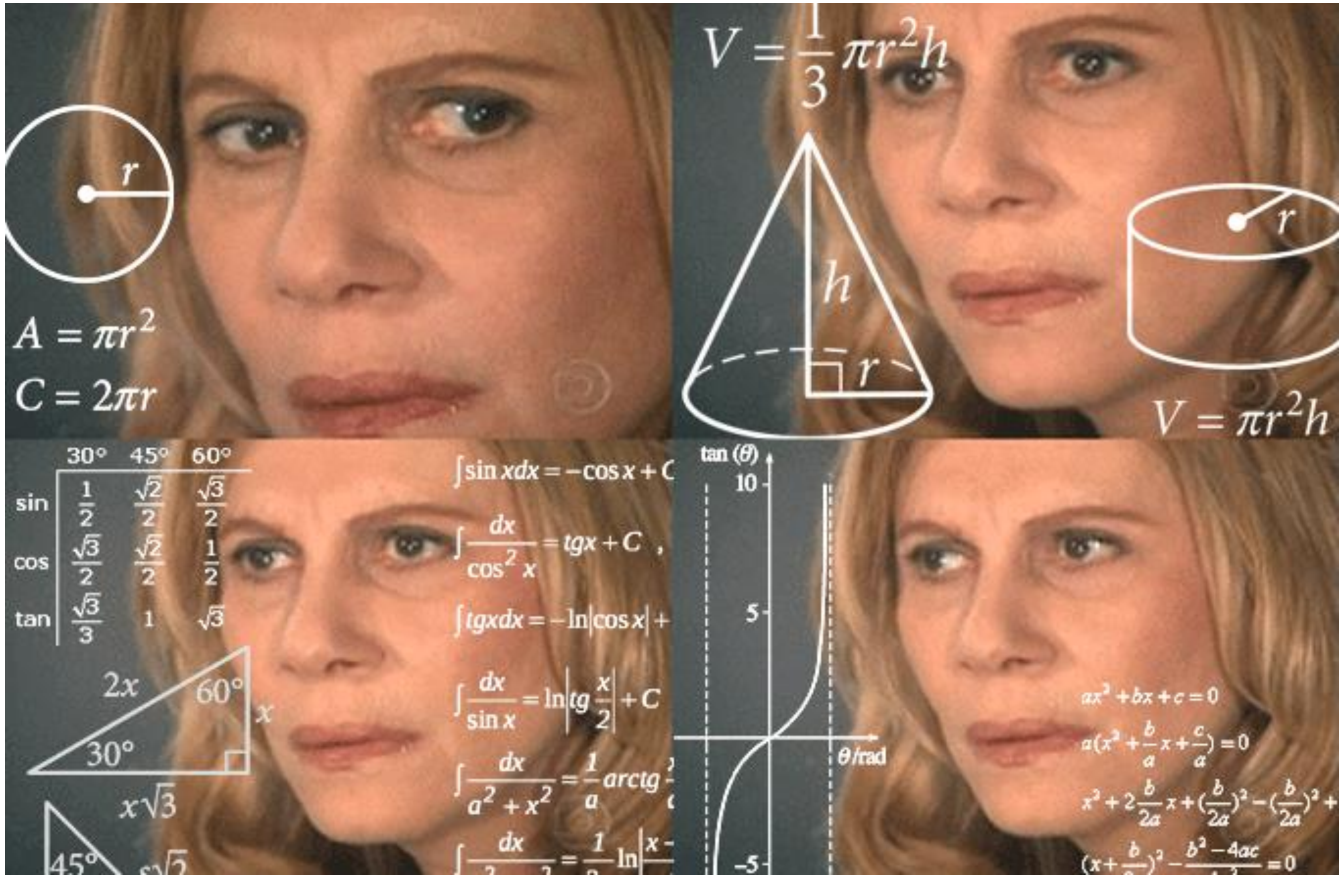
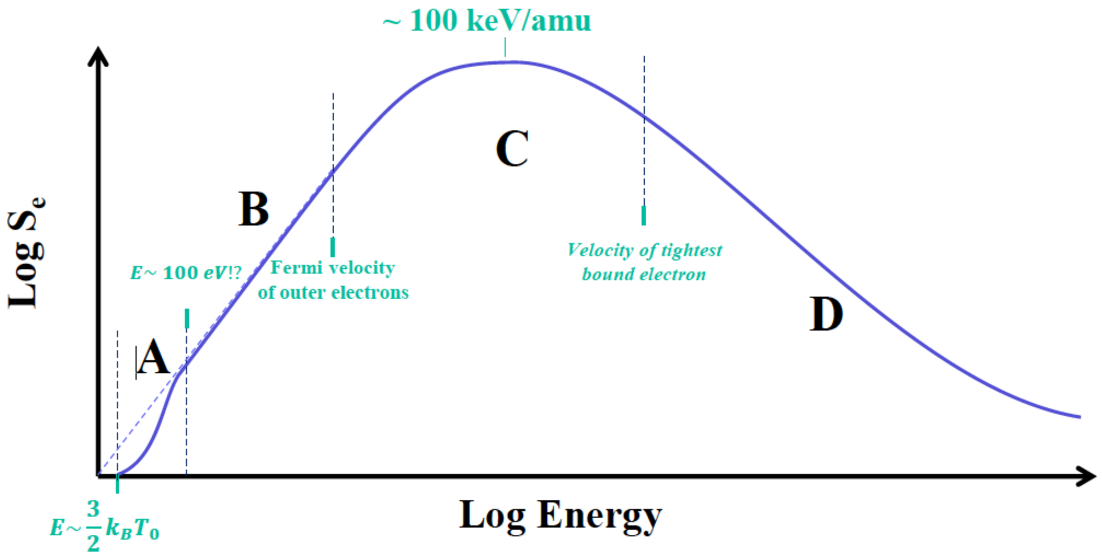
Questions?



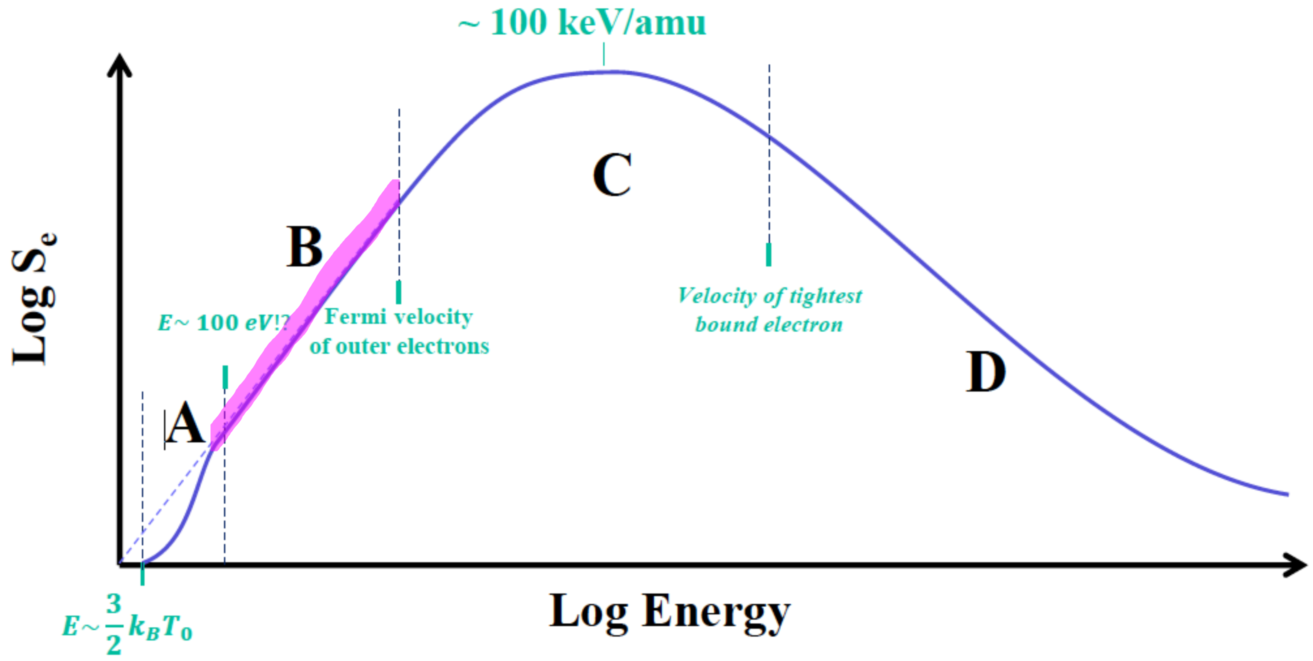
Regime A: low energy regime





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,

$S_e \propto v$

- This regime has an upper limit at the Fermi velocity of the outermost electron of the material
- Regime and derivations agree well with experiments

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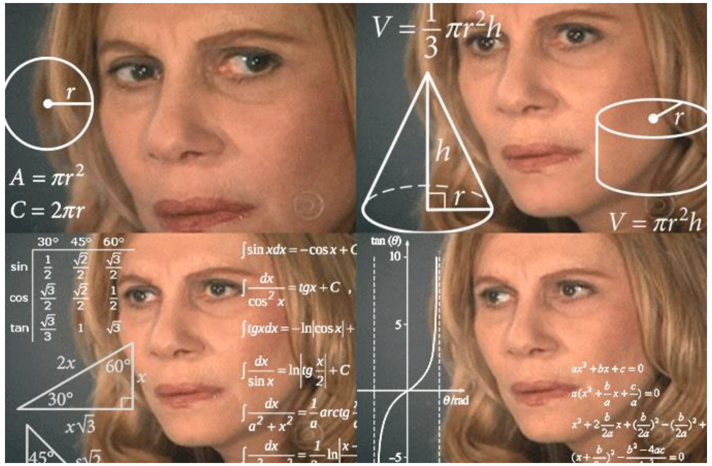
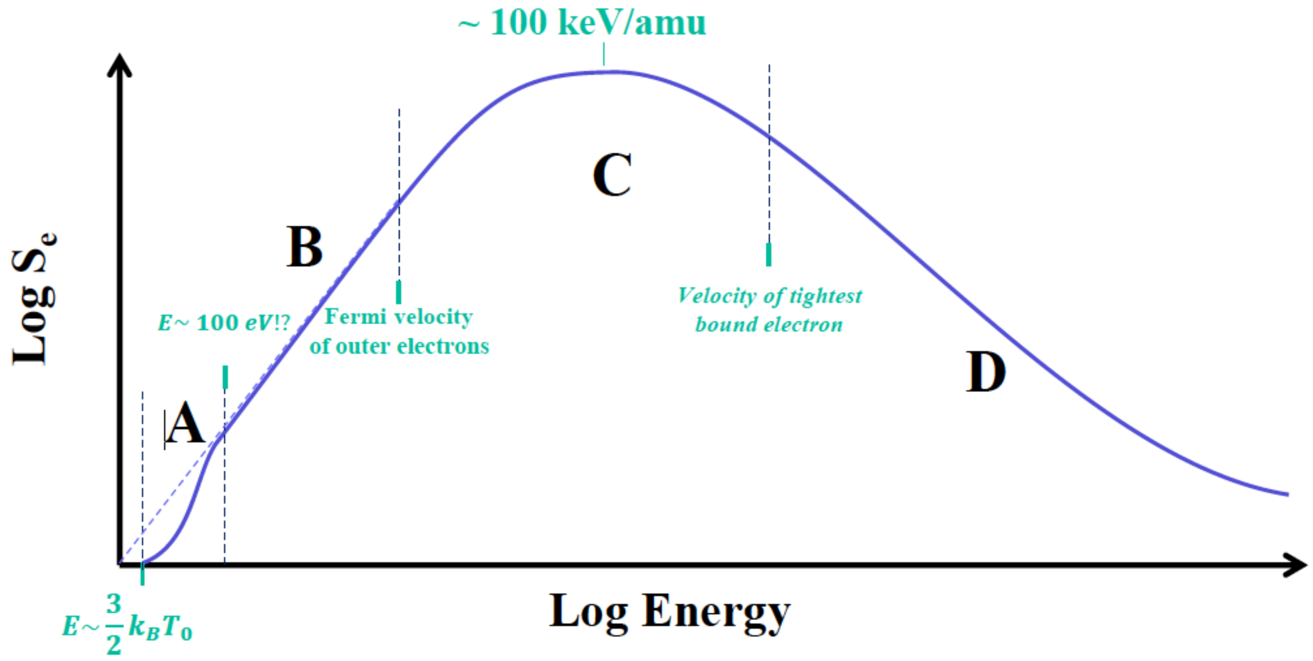
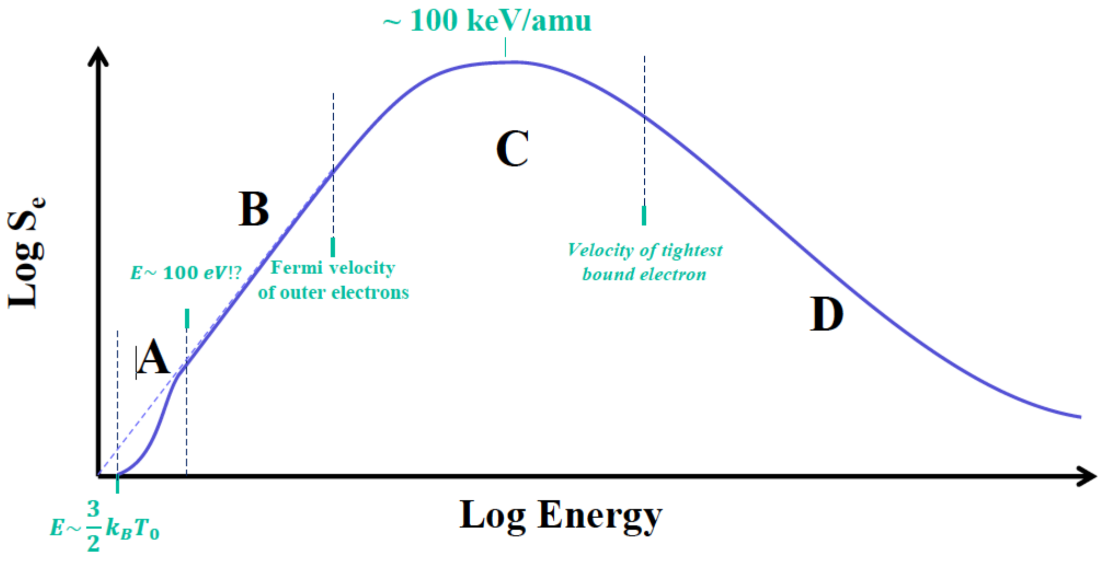
Regime C:





- 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

$$\left(-\frac{\mathrm{d}E}{\mathrm{d}x}\right)_{\mathrm{e}} = \frac{N2\pi Z_1^2 Z_2 \varepsilon^4}{E_{\mathrm{i}}}\frac{M}{m_{\mathrm{e}}}\ln\left(\frac{\gamma_{\mathrm{e}}E_{\mathrm{i}}}{\bar{I}}\right) = \frac{2\pi N Z_1^2 M \varepsilon^4}{m_{\mathrm{e}}E_{\mathrm{i}}}B \qquad B = Z_2 \ln\left(\frac{\gamma_{\mathrm{e}}E_{\mathrm{i}}}{\bar{I}}\right)$$

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