Modifications to K-P Displacement Model & Stopping Powers

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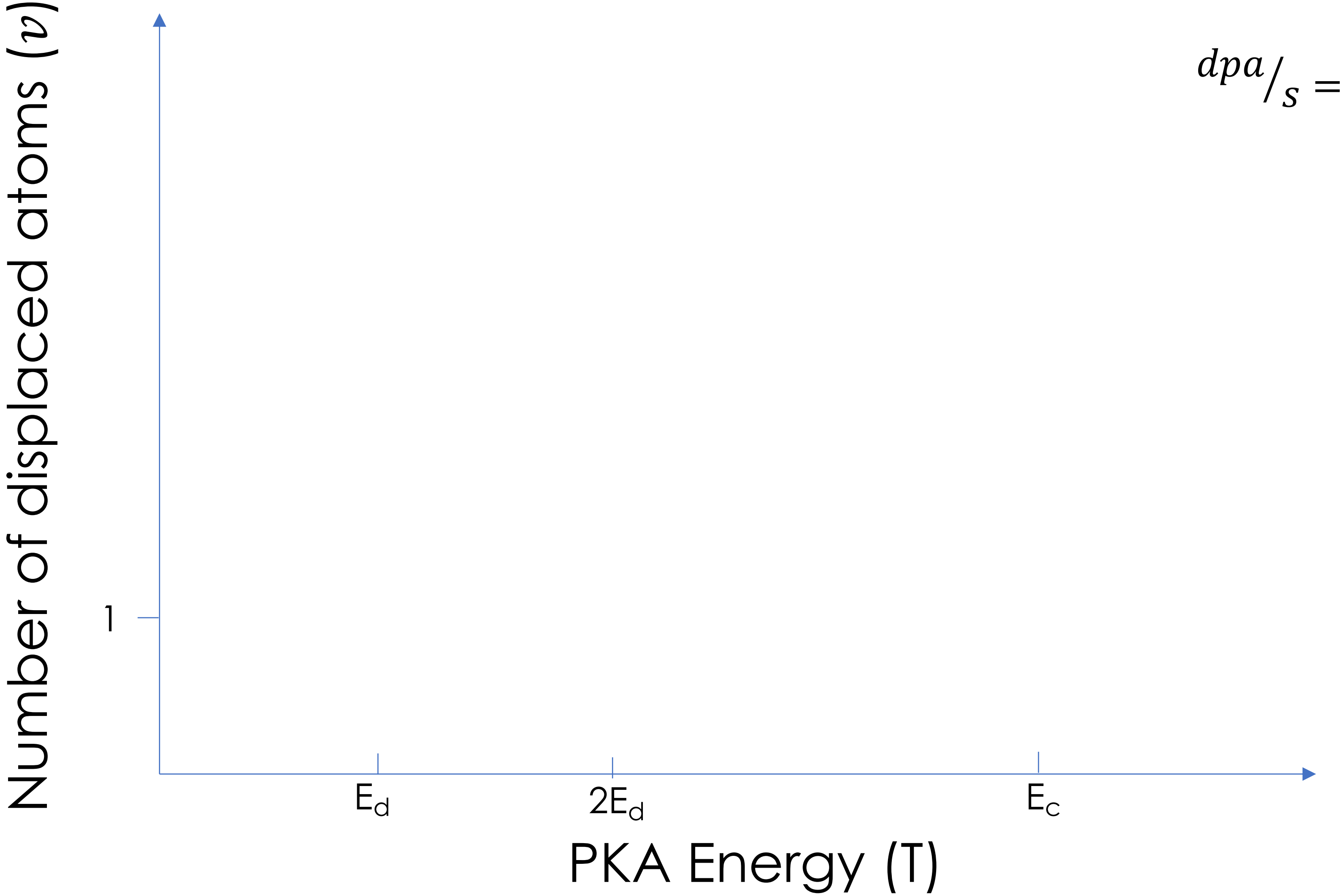
Summary of Topics Covered



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

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Example calculation…

Assume a pure piece of BCC iron is irradiated in a reactor with a monoenergetic flux of 5E13 cm^3/s 1 MeV neutrons. Calculate the time it takes to reach 1 dpa in the iron sample.

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

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Example calculation…

You might find this helpful:

Part I: The radiation damage event

Objective: Develop a fundamental understanding of the physics of the radiation damage event

Day	Date	Lec. #	Topic	Lecture Notes	Assignments	Other resources/details
Tuesday	Aug. 30	1	Introduction	Notes / Recording	-	-
Thursday	Sept. 1	2	Basic particle interactions	Notes / Recording	-	Alt. basic particle derivation
Tuesday	Sept. 6	3	Collision Kinematics	Notes / Recording		Collision Derivation
Thursday	Sept. 8	4	Interatomic Potentials & Cross Sections	Notes / Recording	PS#1	Flux/Fluence/Cross-sections/[illegible]ergy transfer quick review
Tuesday	Sept. 13	5	Simple Disp. Theory		-	Displacement Integrals / [illegible]ersions
Thursday	Sept. 15	6	Energy loss & K-P modifications		-	
Tuesday	Sept. 20	-	Focus, Channel, Range	-	PS1 due	-
Thursday	Sept. 22	7	*No lecture - Prof. Field out of town*			
Tuesday	Sept. 27	8	Damage Cascades		PS#2	Arc-dpa Paper

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Example calculation…

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

A simple picture of slowing down

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

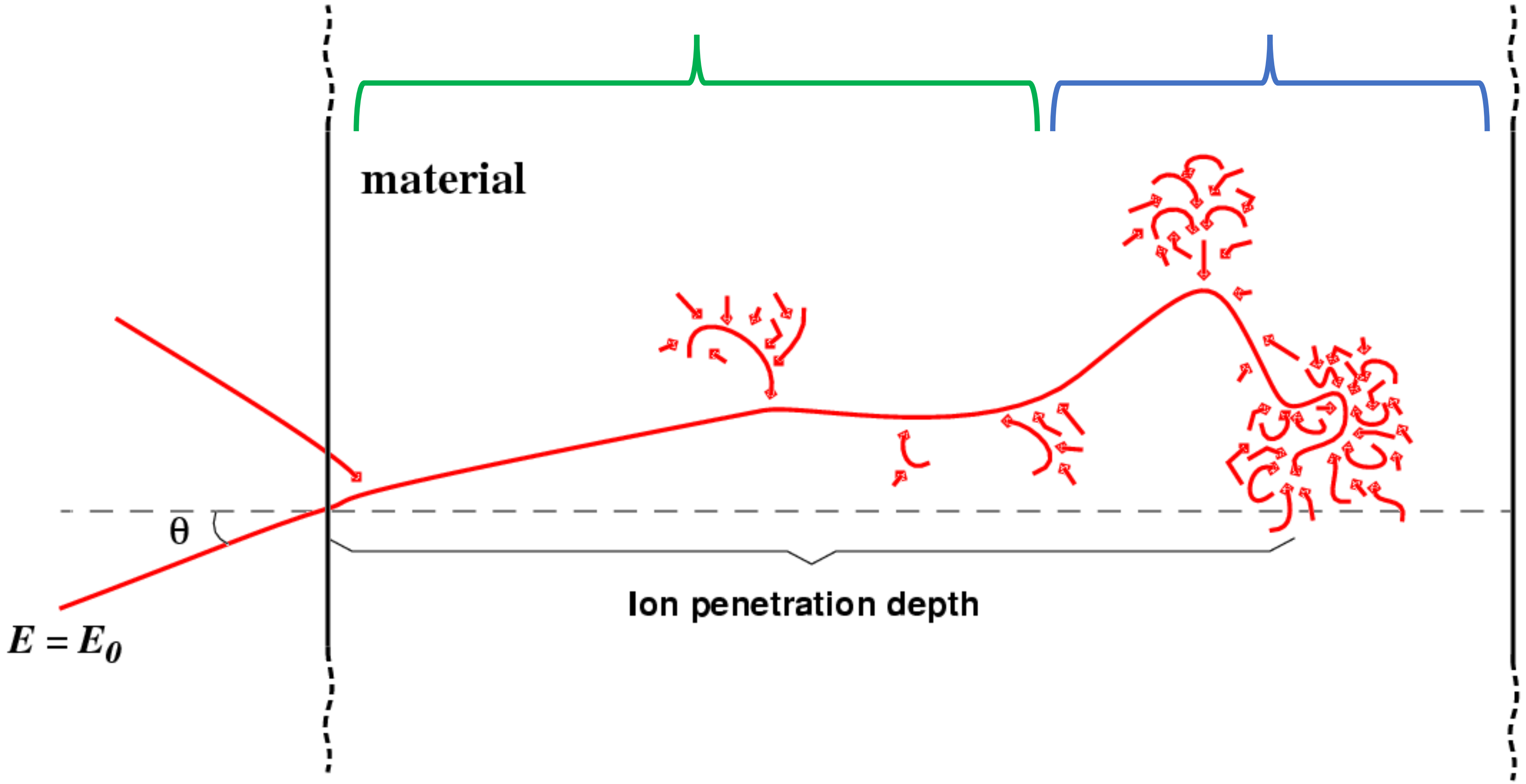
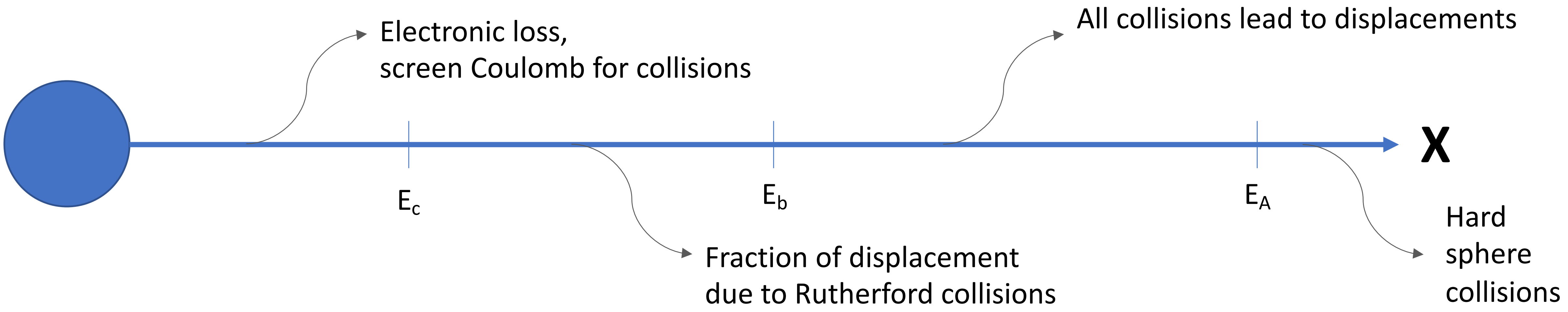


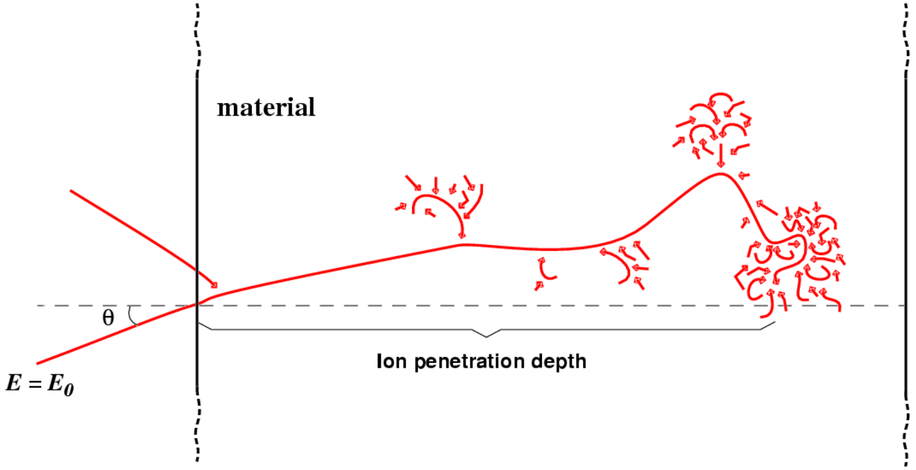
Image: Kai Nordlud

Regimes of energy loss of a PKA



The concept of stopping power

- Since the electronic collisions only slow down the ion, 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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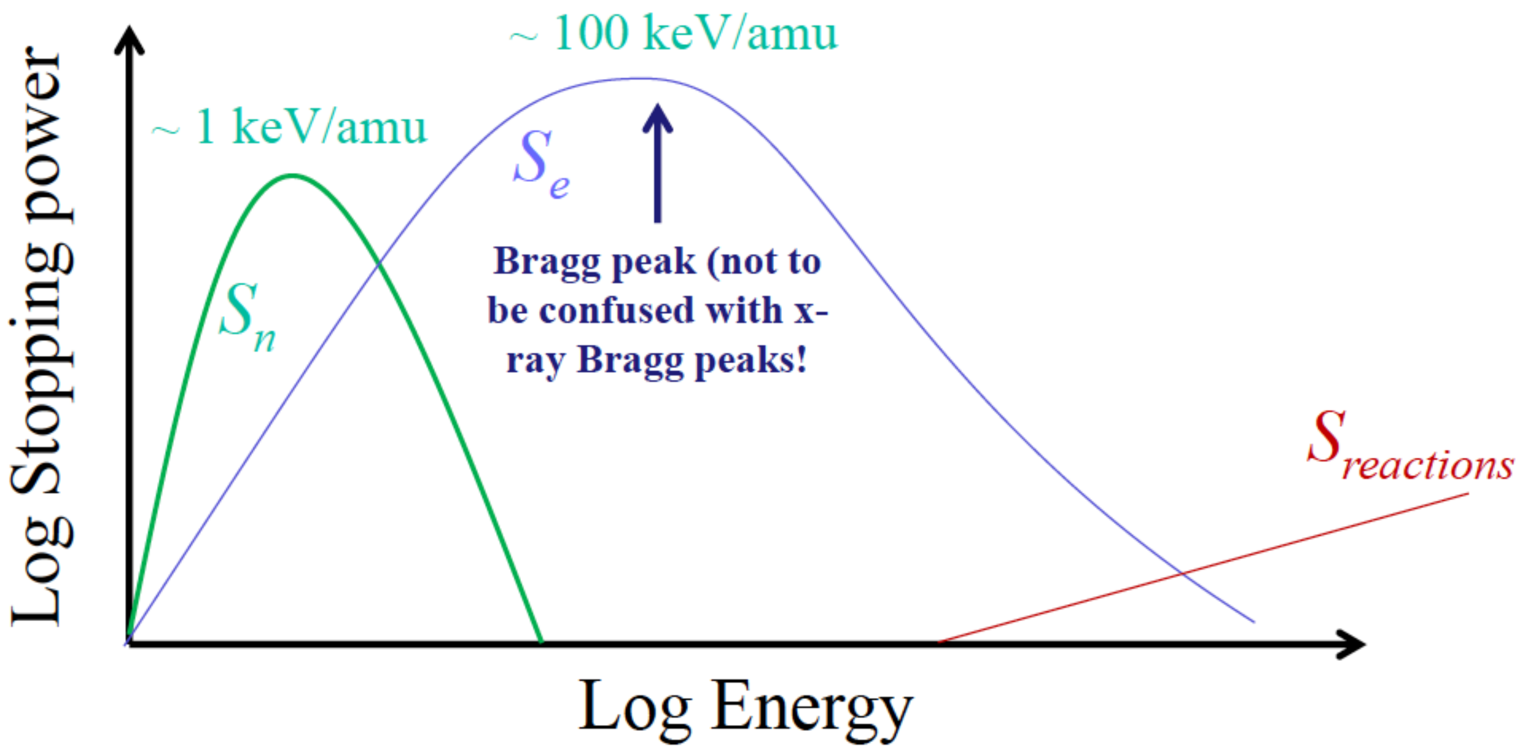
Stopping power

- The total stopping power can be written as

- Schematically, the energy dependence of these is then:



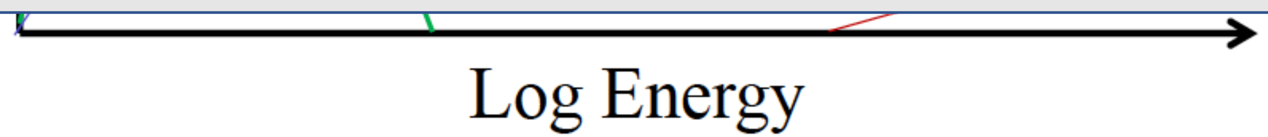
Slide: Kai Nordlud

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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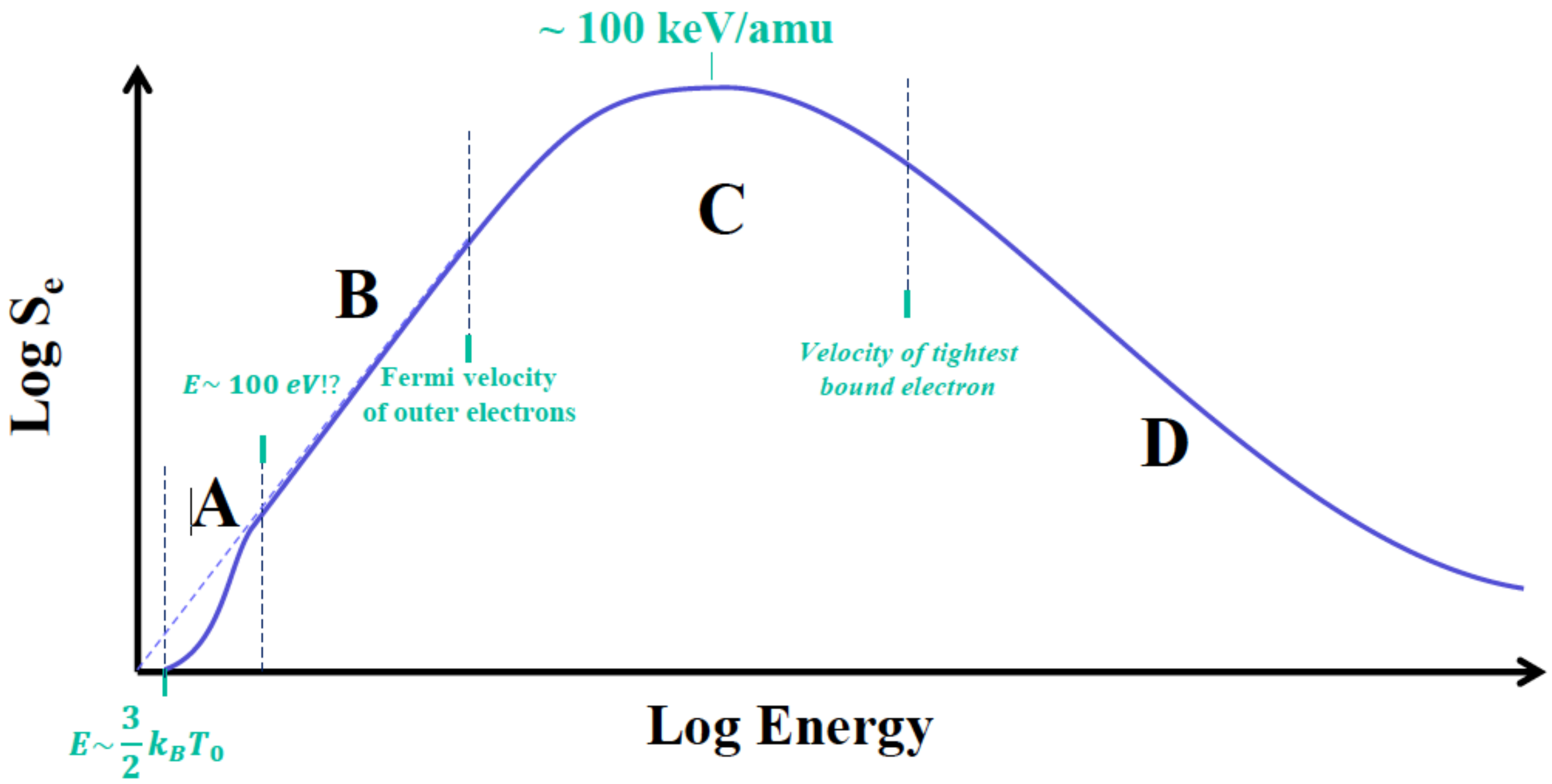
Regimes of electronic stopping power

- Electronic stopping can be segregated into four primary regimes:



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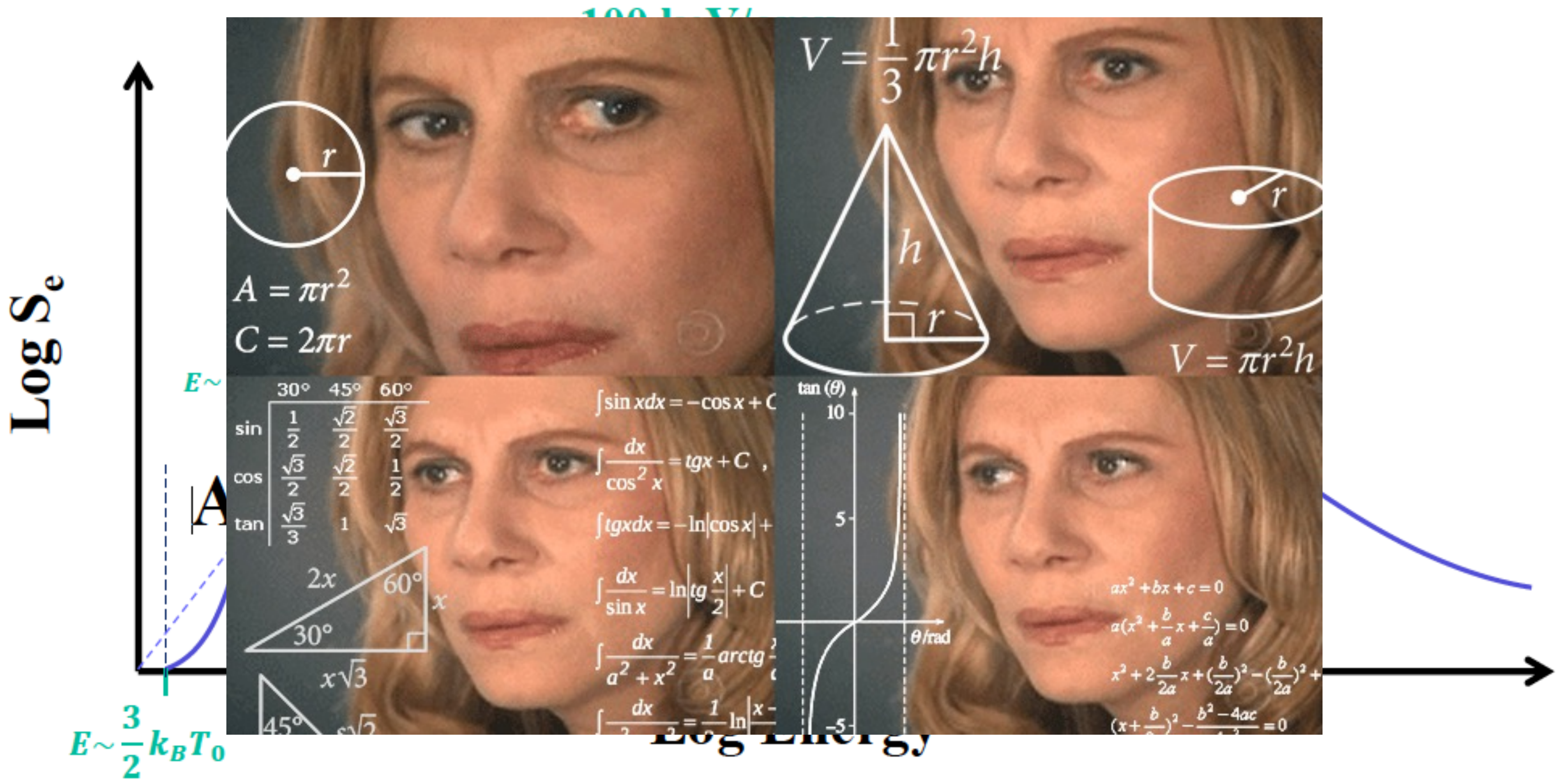

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Stopping powers

- $\left(-{}^{dE}/_{dx}\right)_{total}$ can be written in terms of stopping power (units of energy * distance²):

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

- 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:

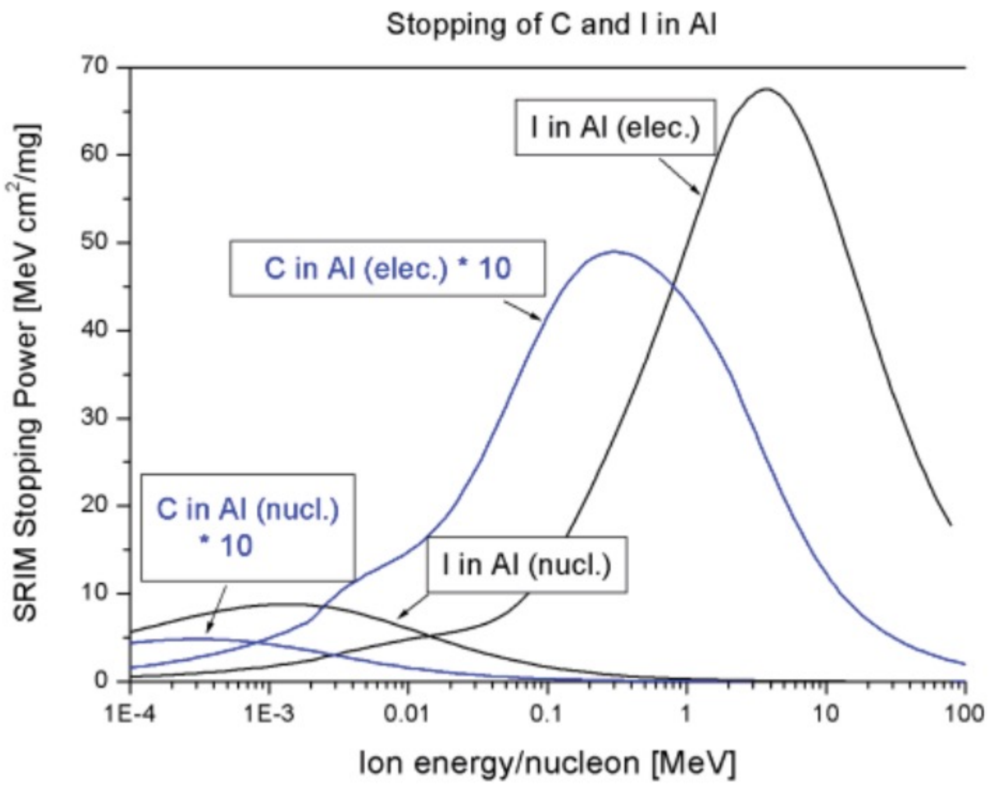

FIGURE 2. Electronic and nuclear mass stopping power for carbon and iodine ions in aluminum, calculated using SRIM.

- Electronic stopping power dominates for high energy ions

https://doi.org/10.1063/1.4802339

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 $K=\left(\frac{\pi}{e}\right)\varepsilon^2a_0=2.8\times10^{-15}\ \mathrm{eV\cdot cm^2}$	(1.163)	$k=8\sigma_eN\left(\frac{m_e}{M_1}\right)^{1/2}$ valid for $0 < E\ (keV) < 37Z^{7/3}$	

Lecture Break

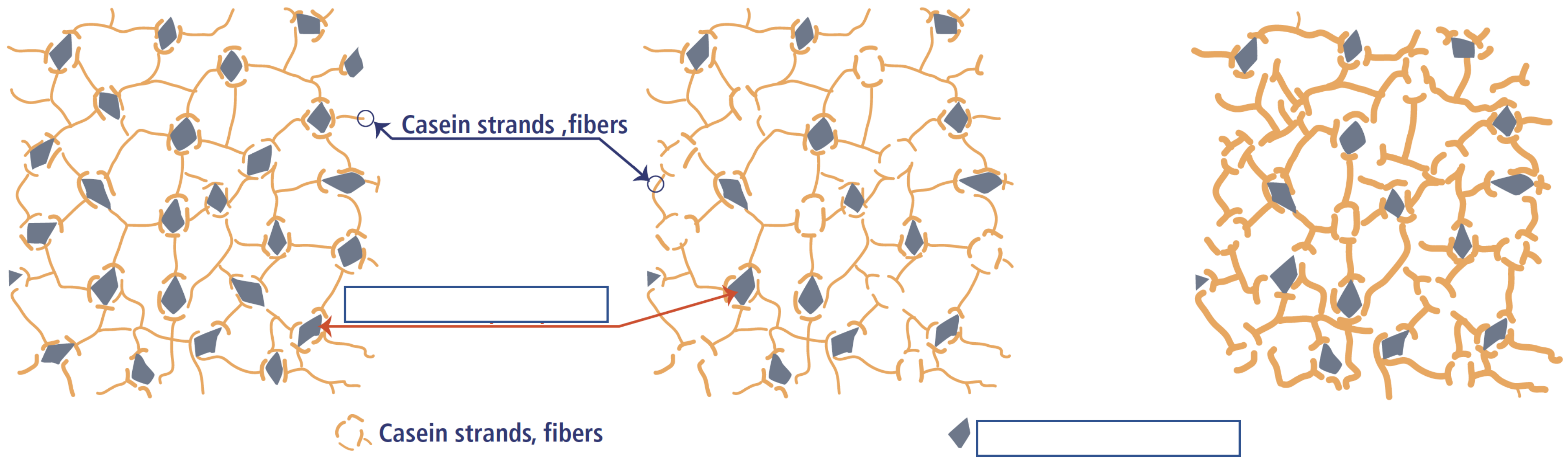
According to Johnson and Polowsky (2016) what is the chemical compound in cheese curds that leads to the “squeak” or effectively the resistance of the casein (protein) to mechanical load when you bite them? Note, this compound dissolves due to the latic acid in the curd over time leading to a loss of the squeak after ~3-5 days.

FIGURE 1: Insoluble in a key crosslinking material in the cheese matrix

Cheese with a high insoluble very interconnected protein matrix, **squeaky.**

Same cheese but with a low content: less interconnected protein matrix, **not squeaky.**

Heated curd microstructure with active and connected protein matrix, **squeaky.**



M. Johnson & P. Polowsky, “Cheese Curds: A Wisconsin Icon” *Dairy Pipeline*, Volume 28:3, 2016

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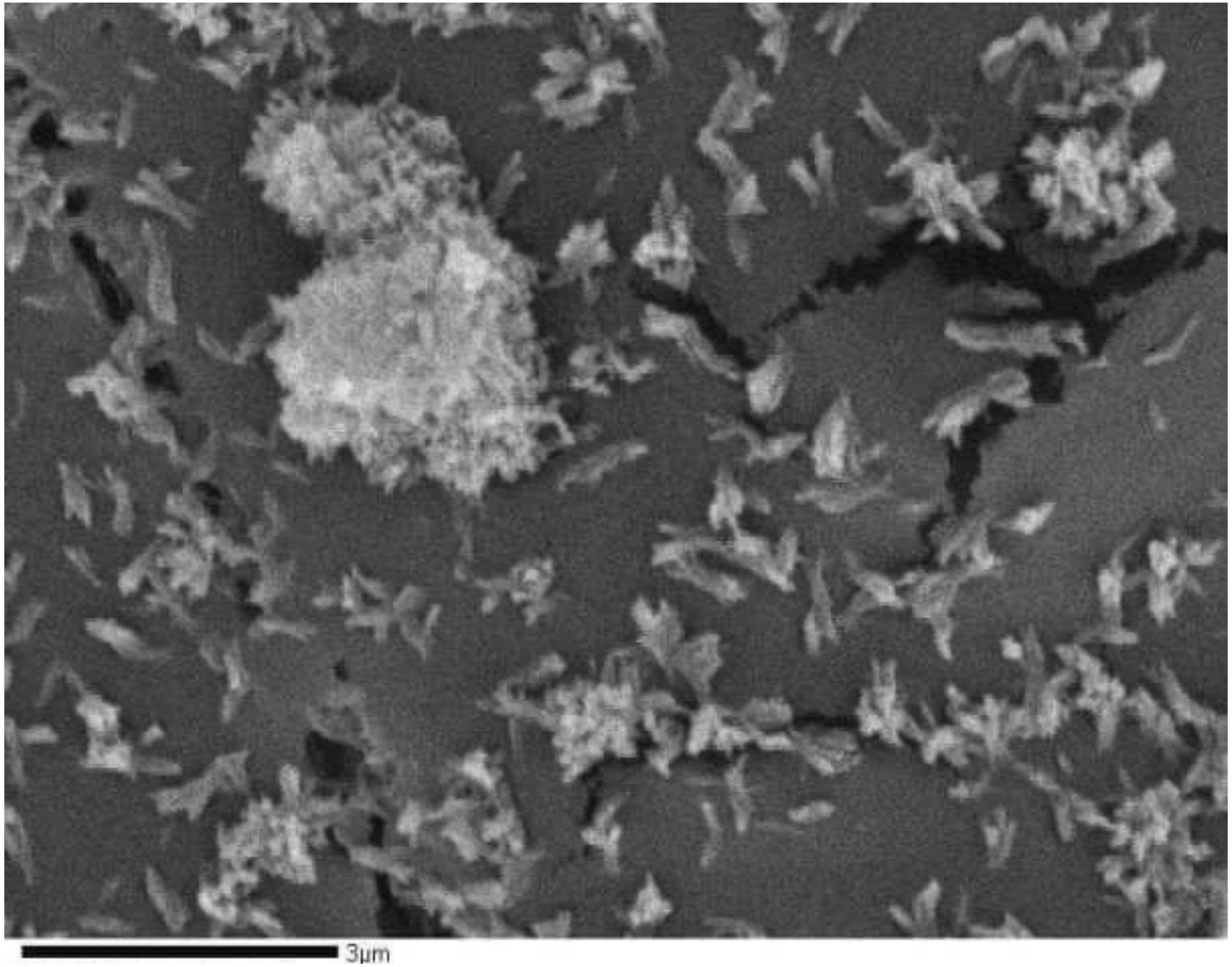
Lecture Break



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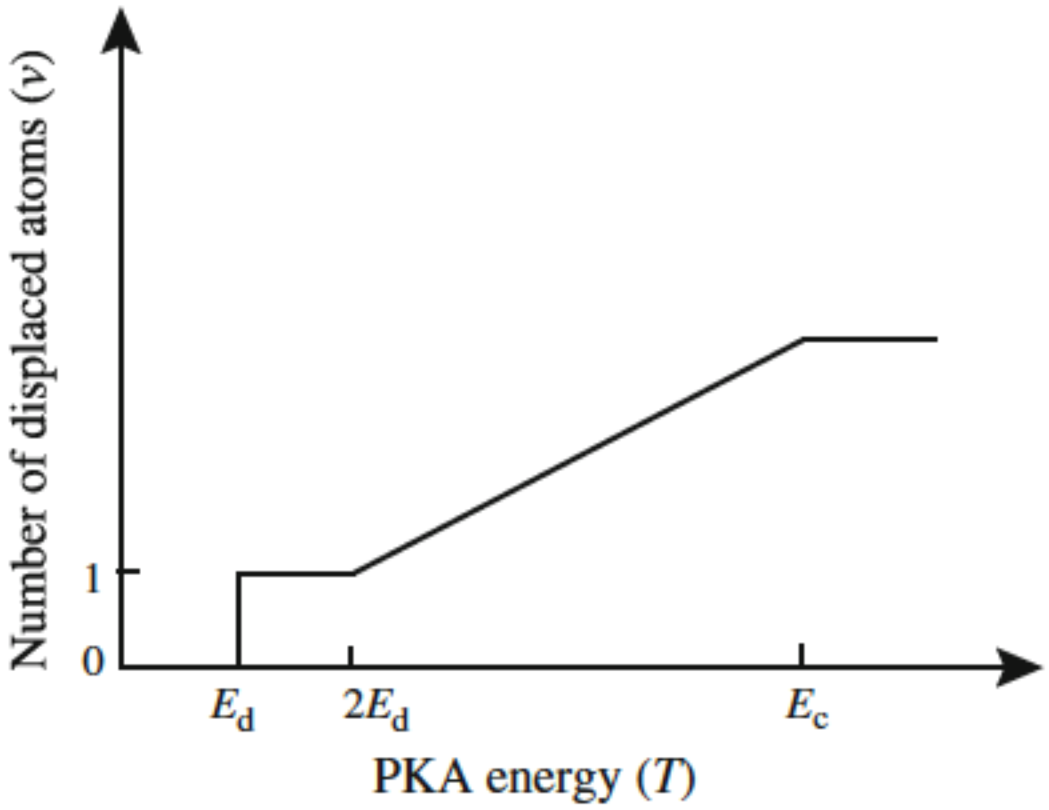
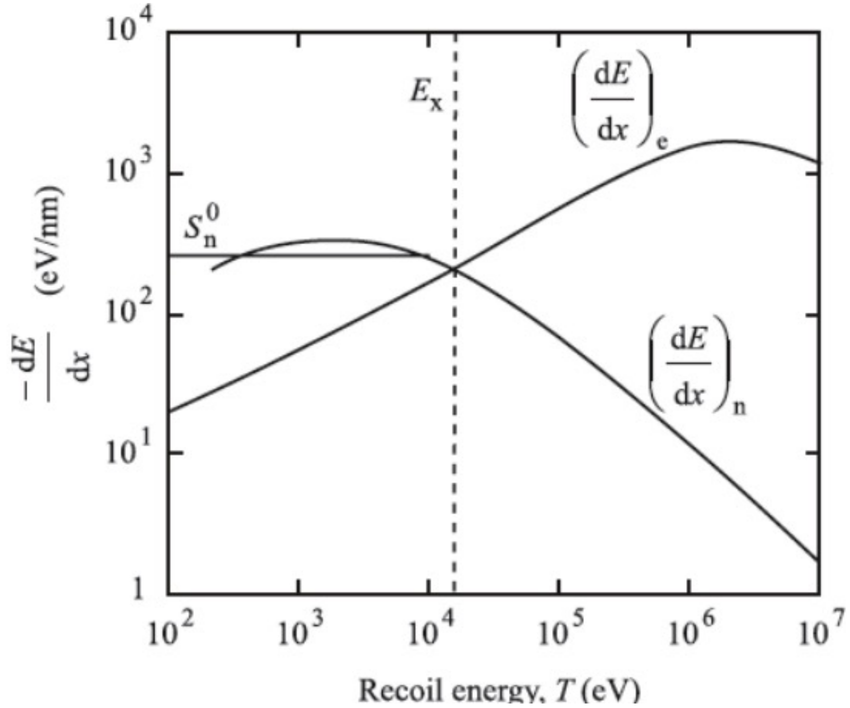
Modifications to K-P Model

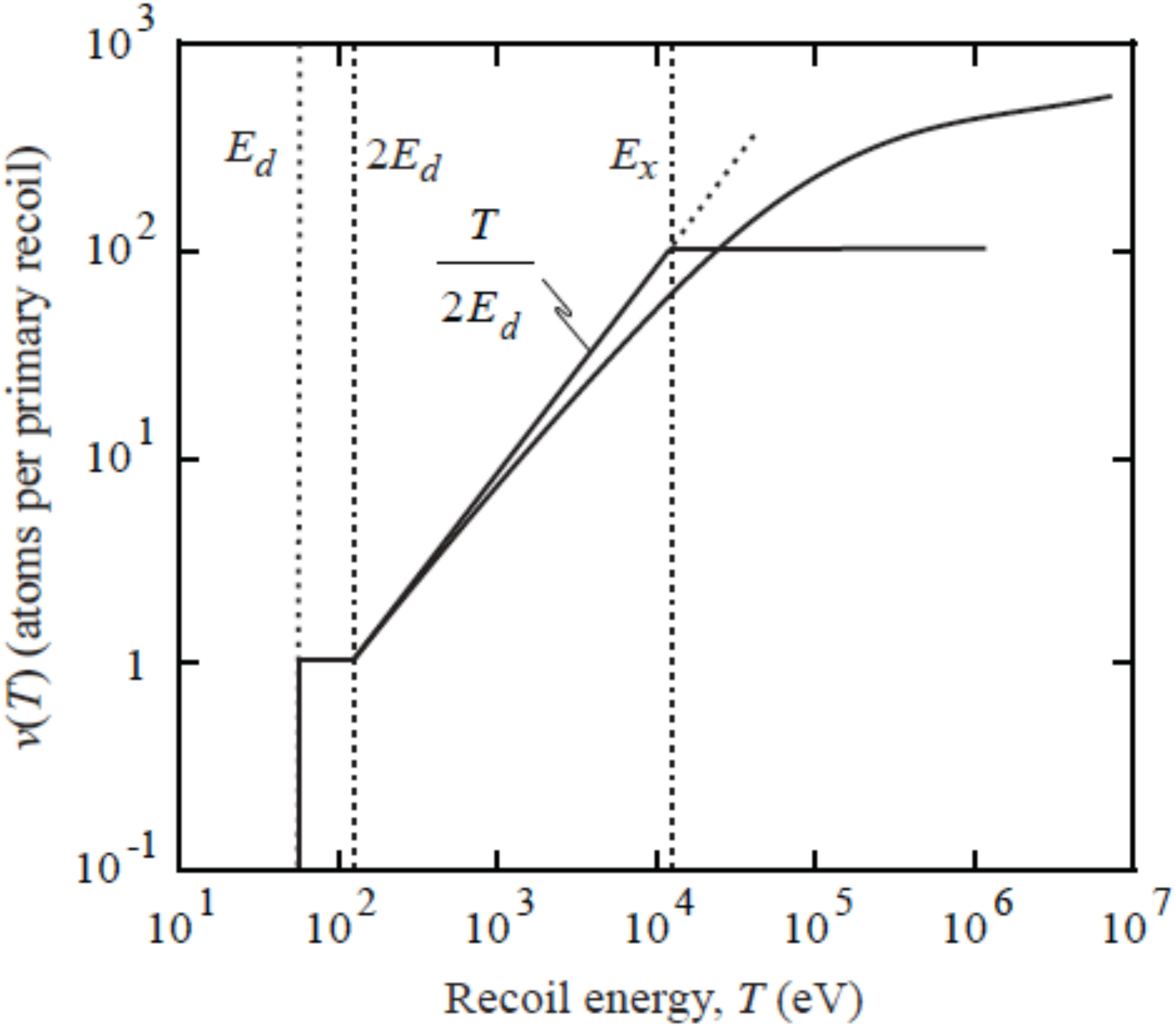
- Many factors to consider (and covered in text), but three are the most important:
    1. Correction for electron energy loss
    2. Use of a realistic cross-section
    3. Effect of crystallinity



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

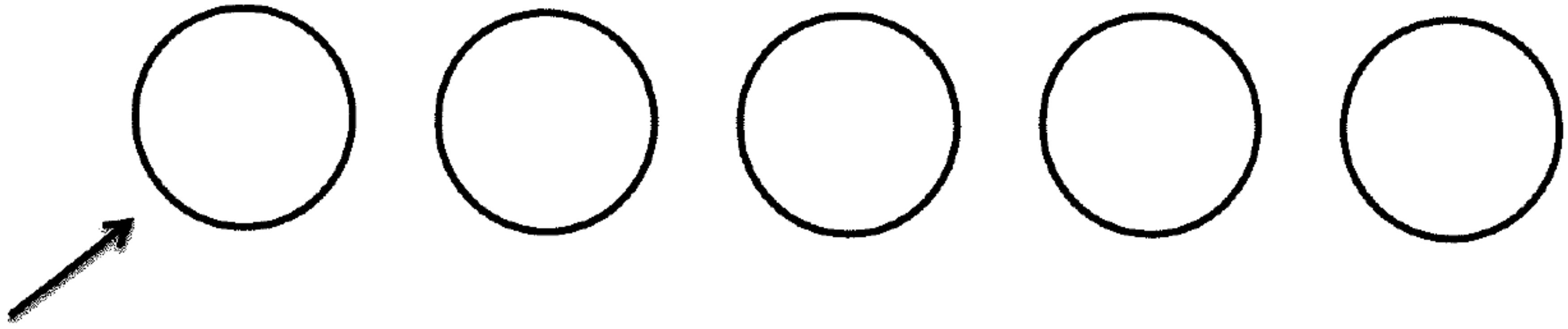




Modifications to K-P Model

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

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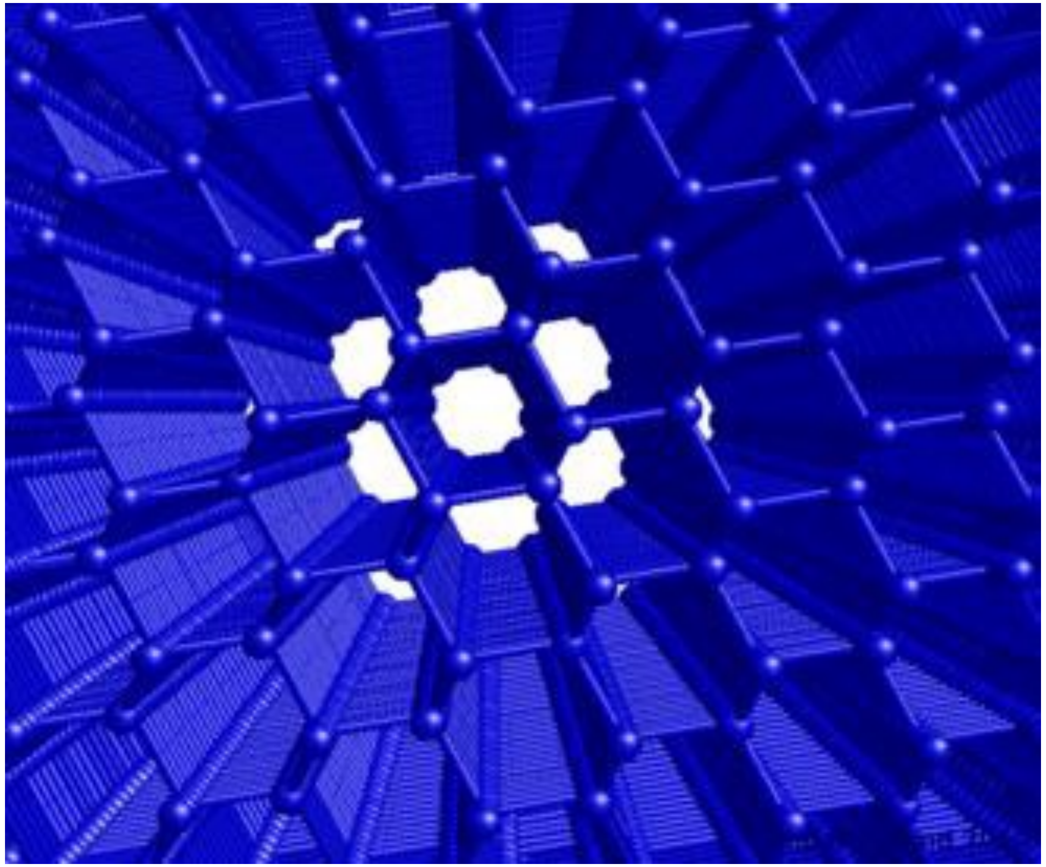
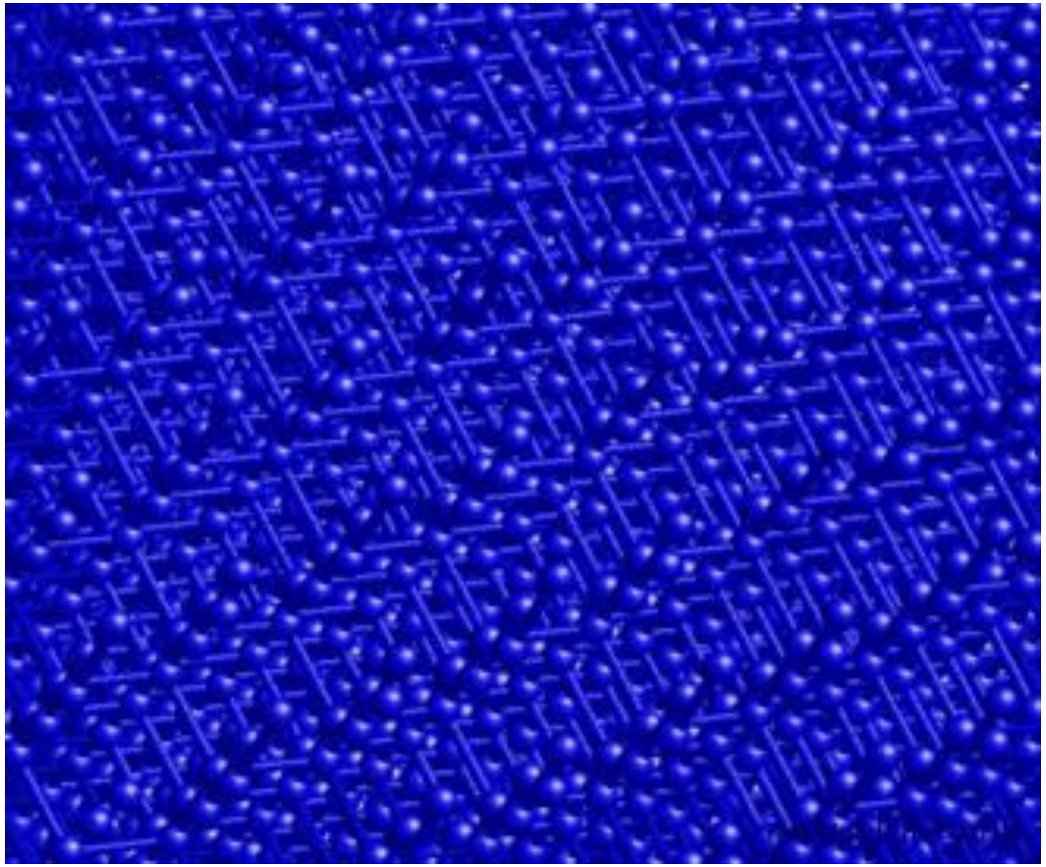
Channeling



Down a primary zone axis



Down a random orienation

Images from Kai Nordlund

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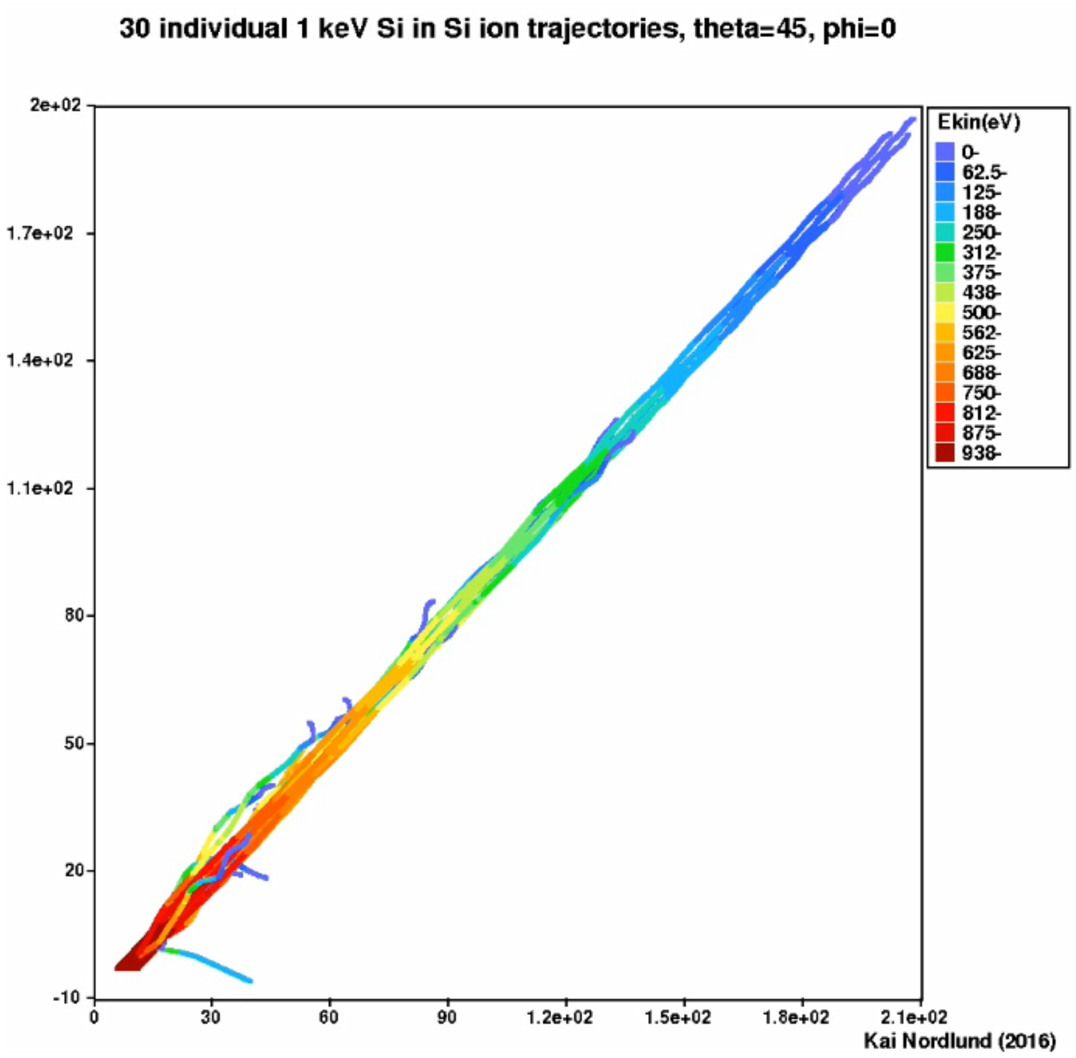
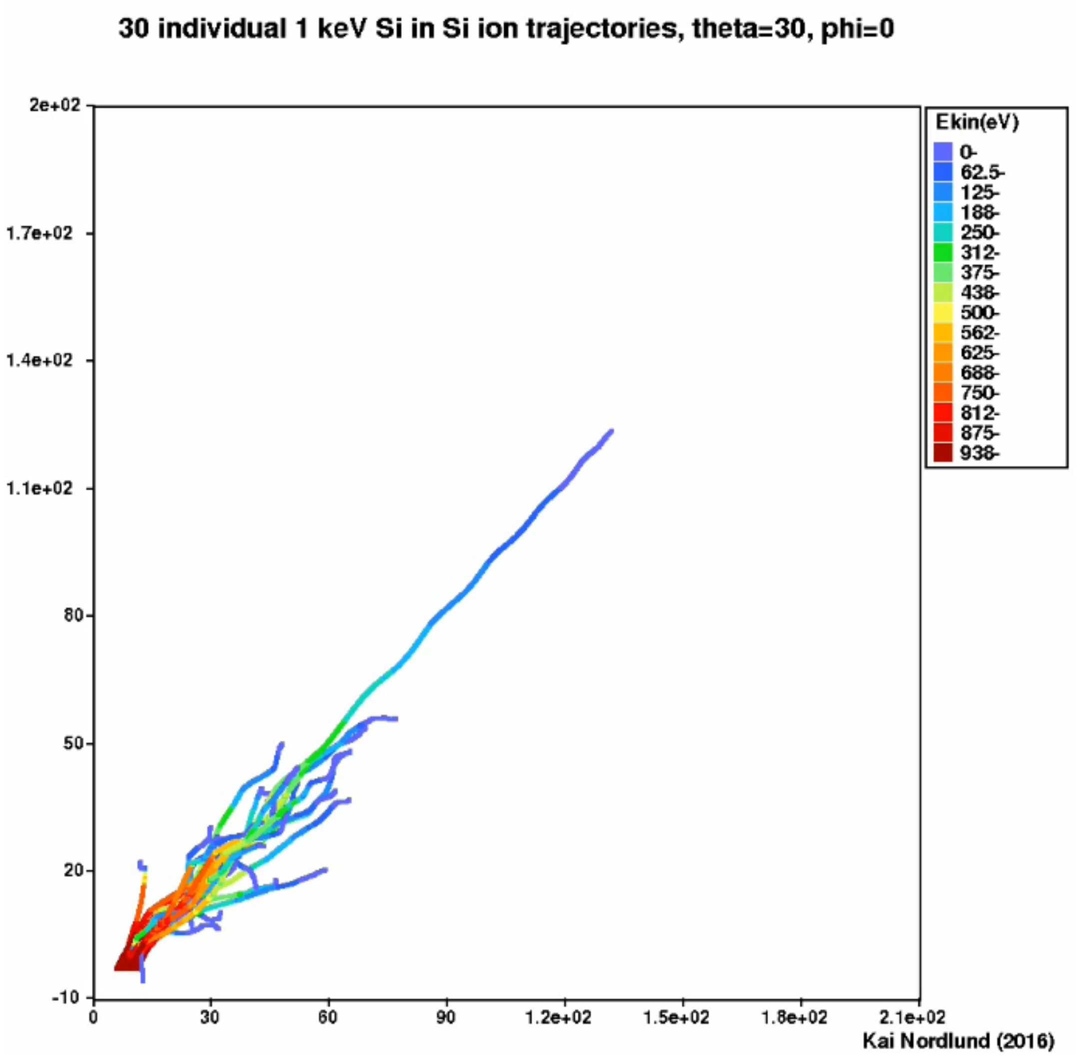
Channeling illustration





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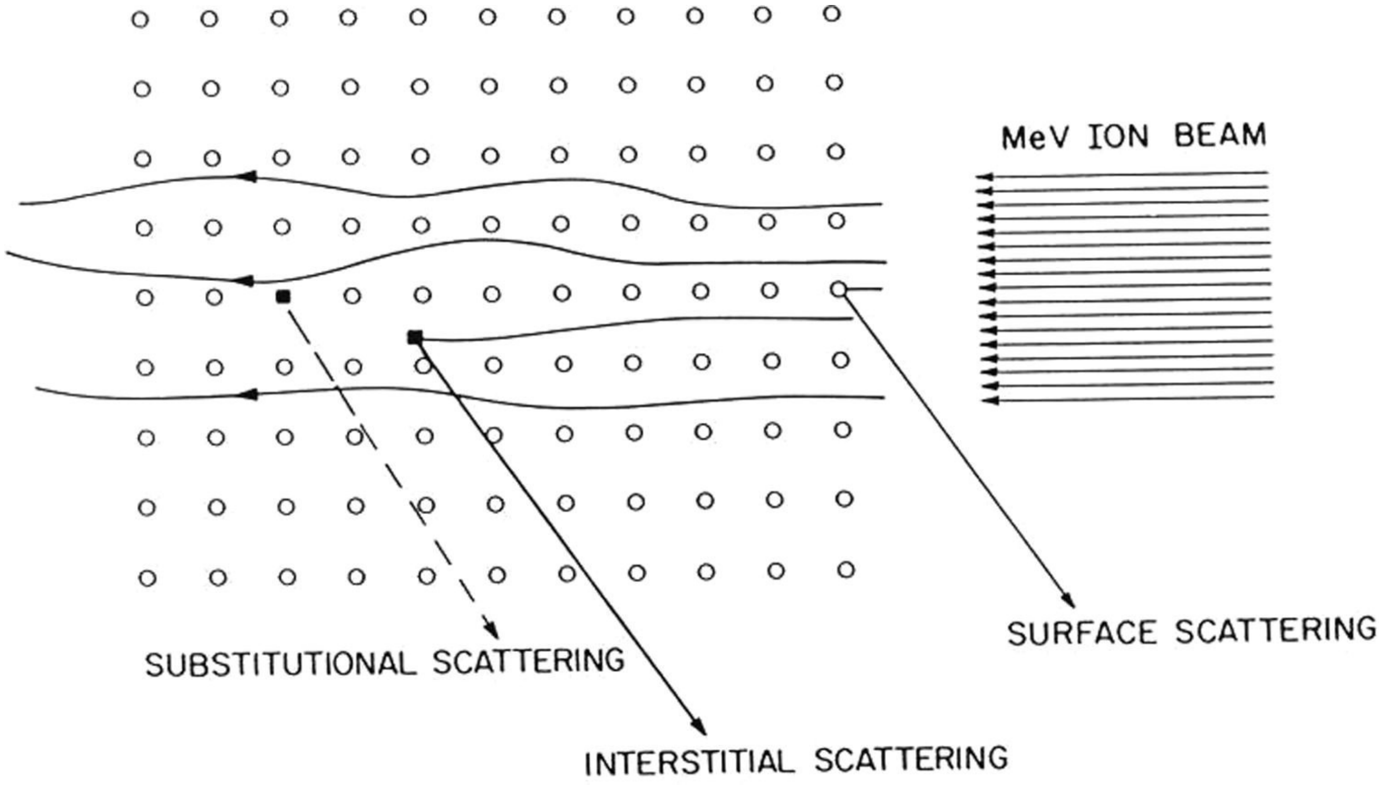
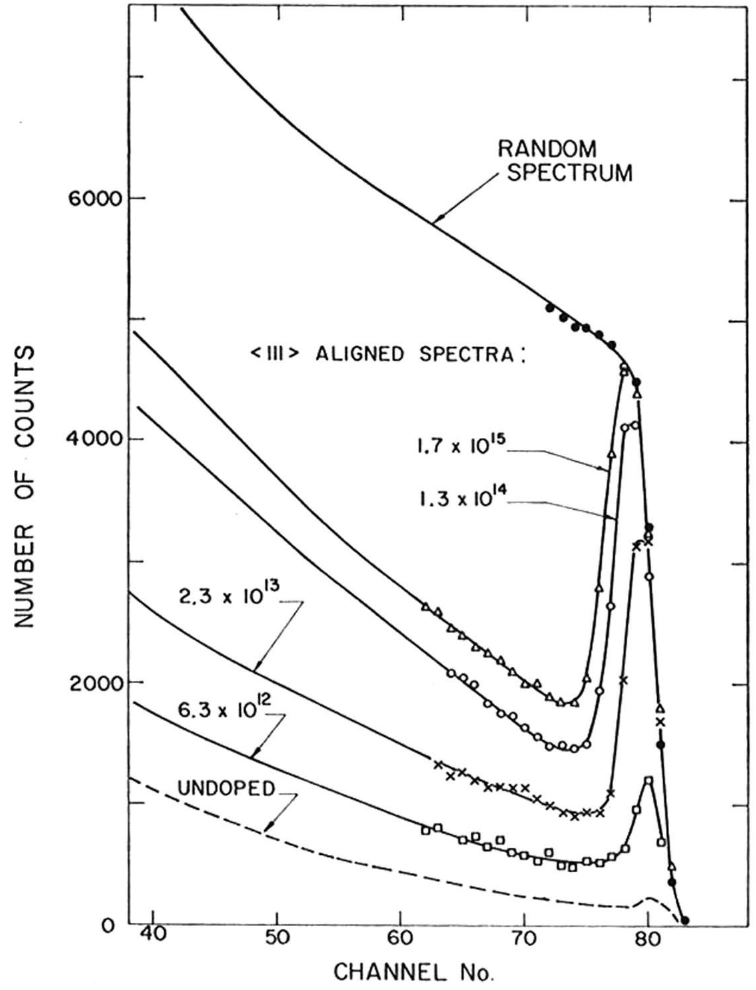
Practical Applications of Channeling





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

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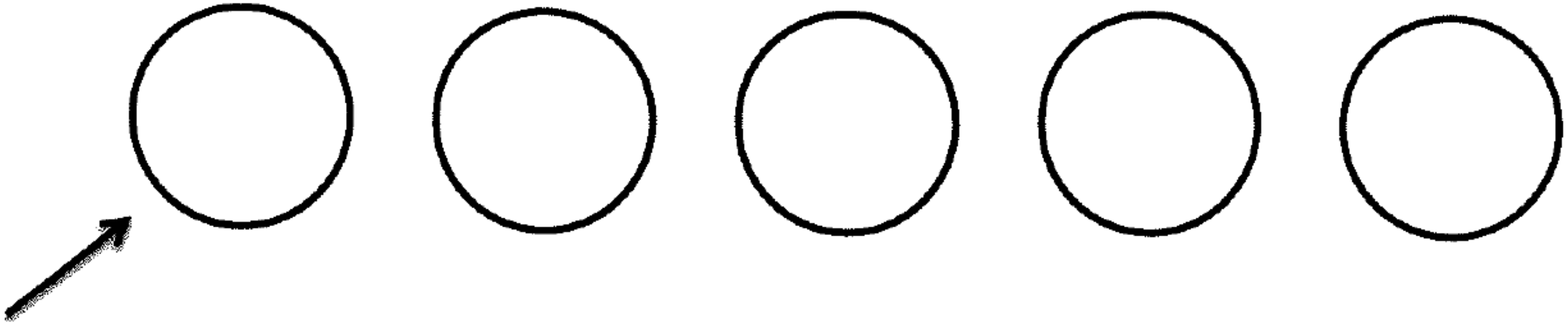
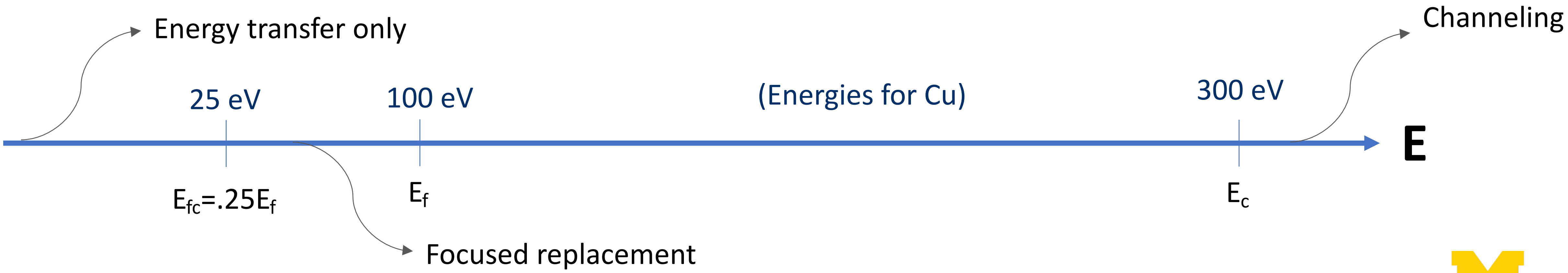
Focusing



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



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Coming back to determining v(T)

Assumption	Correction to $v(T)$	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	$C\frac{T}{2E_d},\ 0.52 \le \mathrm{C} \le 1.22$	(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!!!

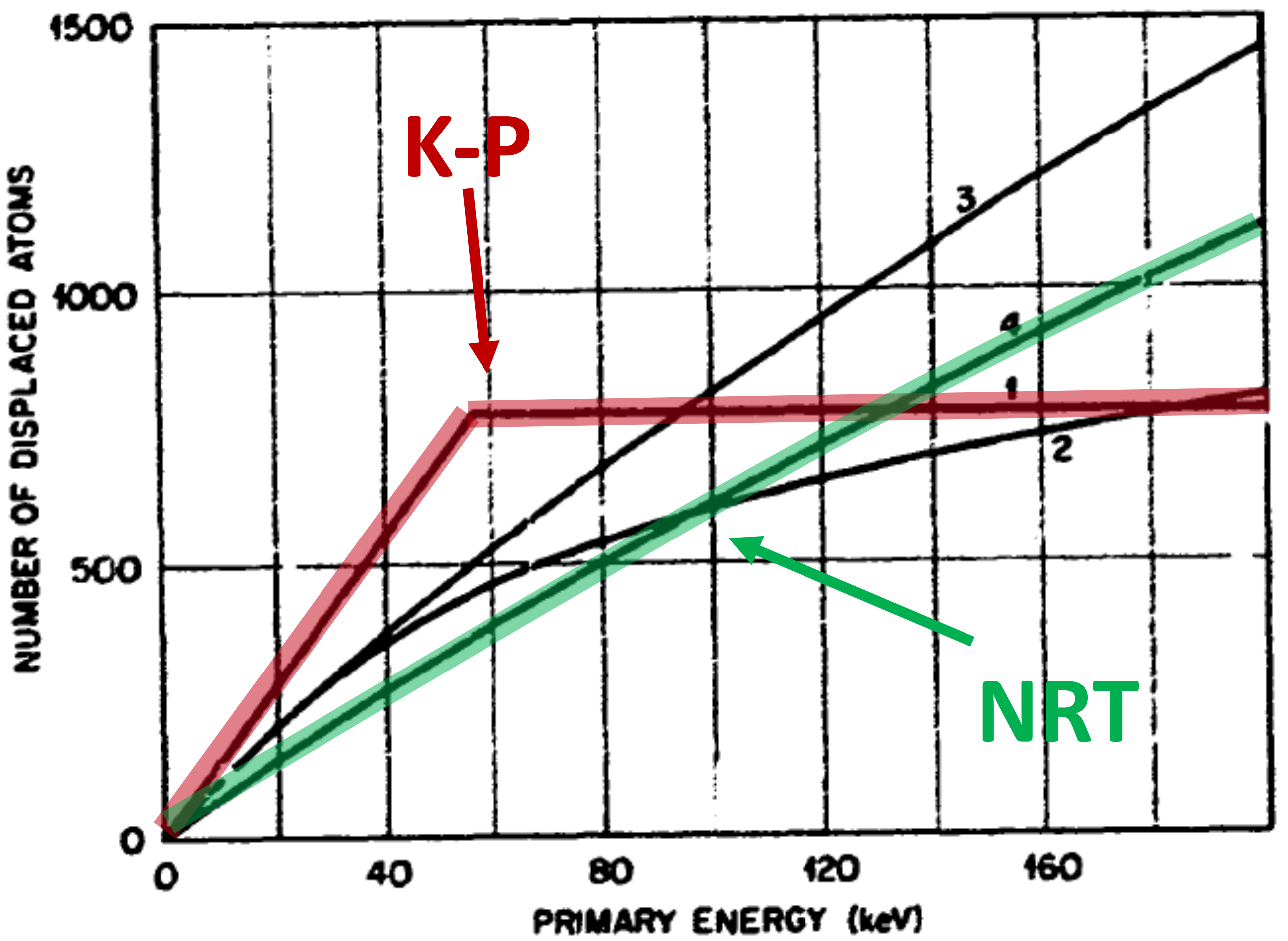

Fig. 2. Comparison of number of displaced atoms generated in bcc iron by a primary knock-on atom. Calculated results correspond to: (1) Kinchin–Pease model with E_d = 40 eV and E_1 = 56 keV; (2) the half-Nelson formula [4]; (3) earlier computer calculations of Norgett [18], using Torrens–Robinson computer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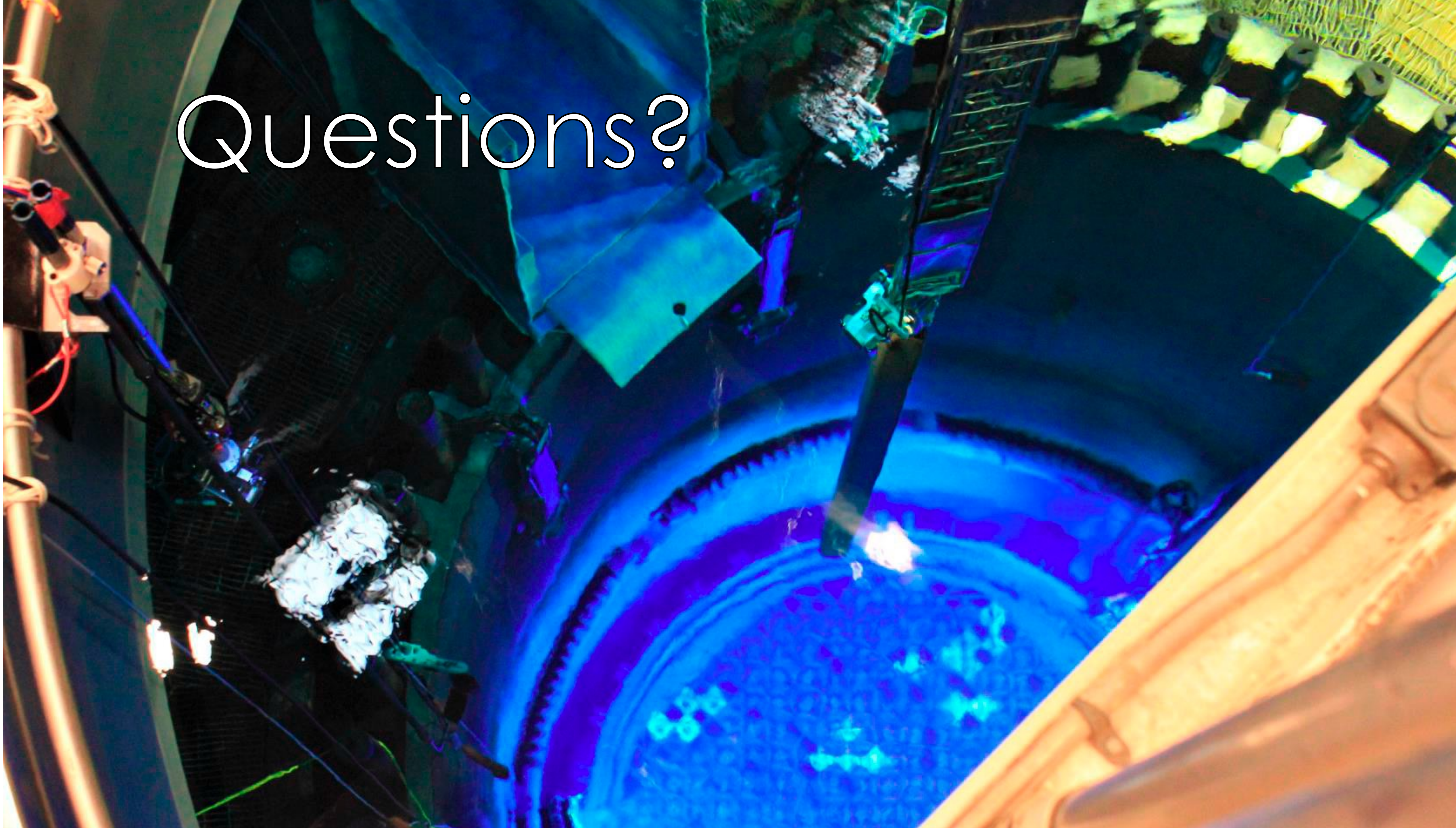
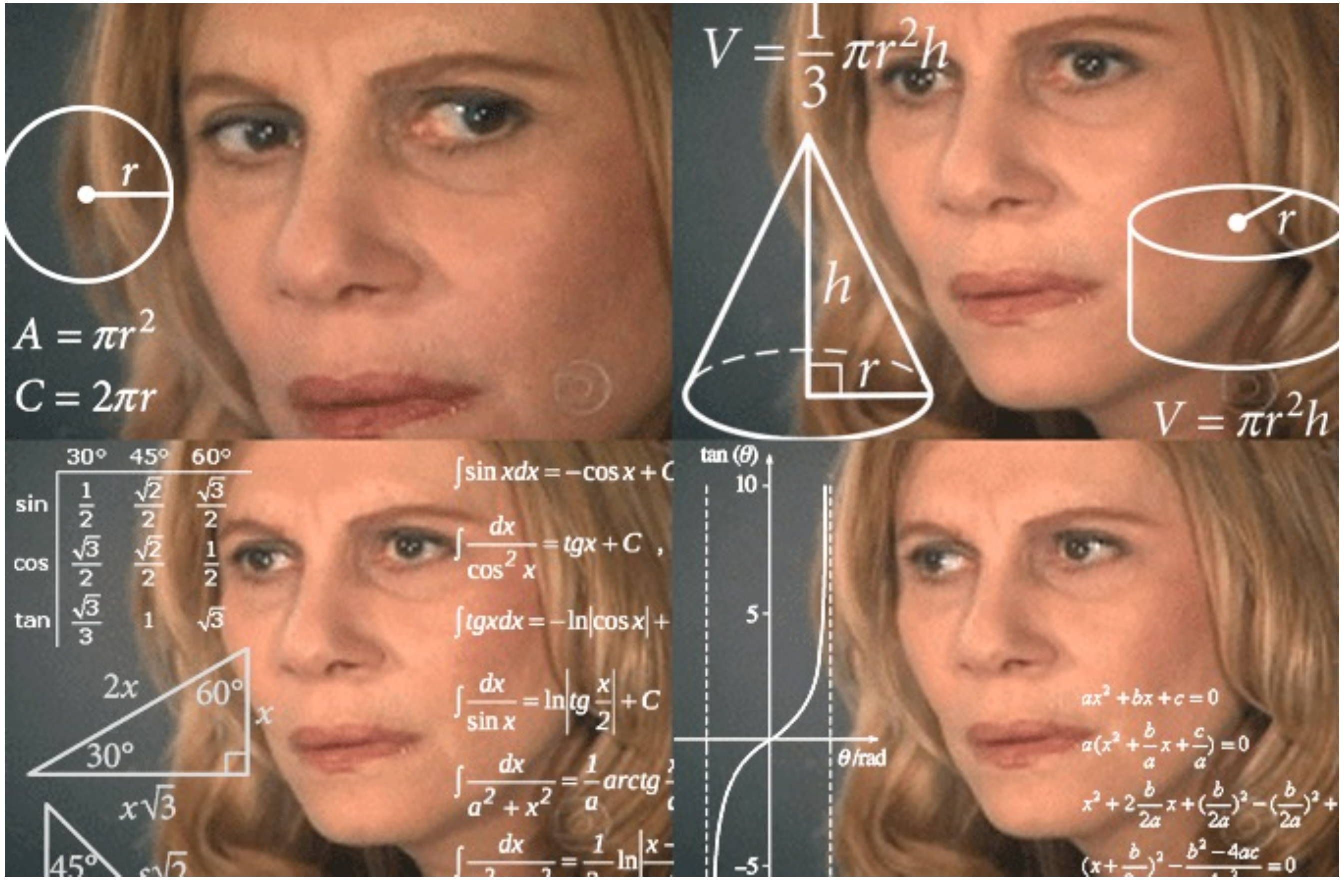
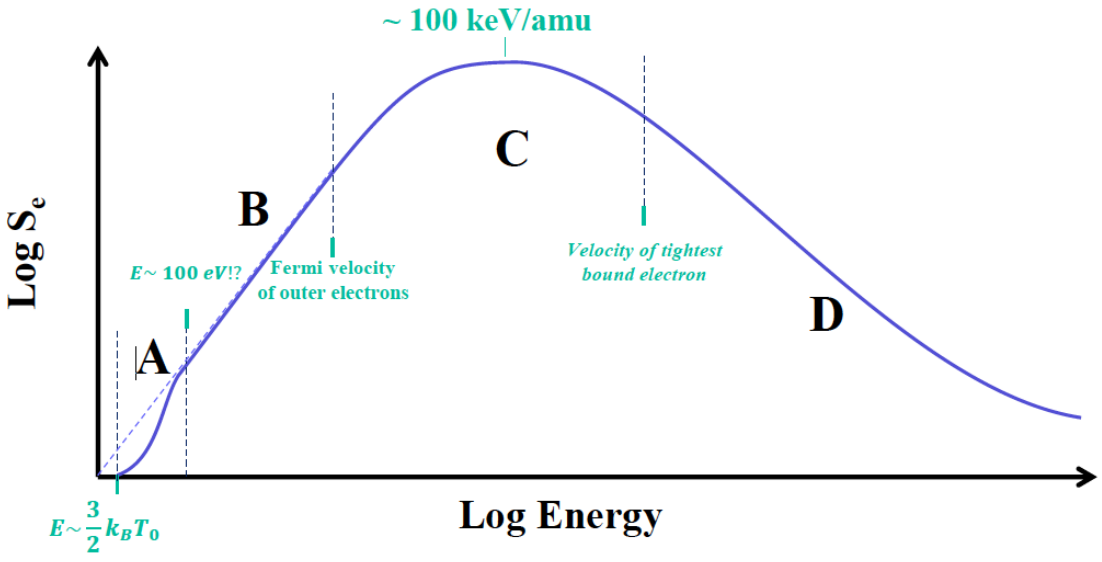

Questions?

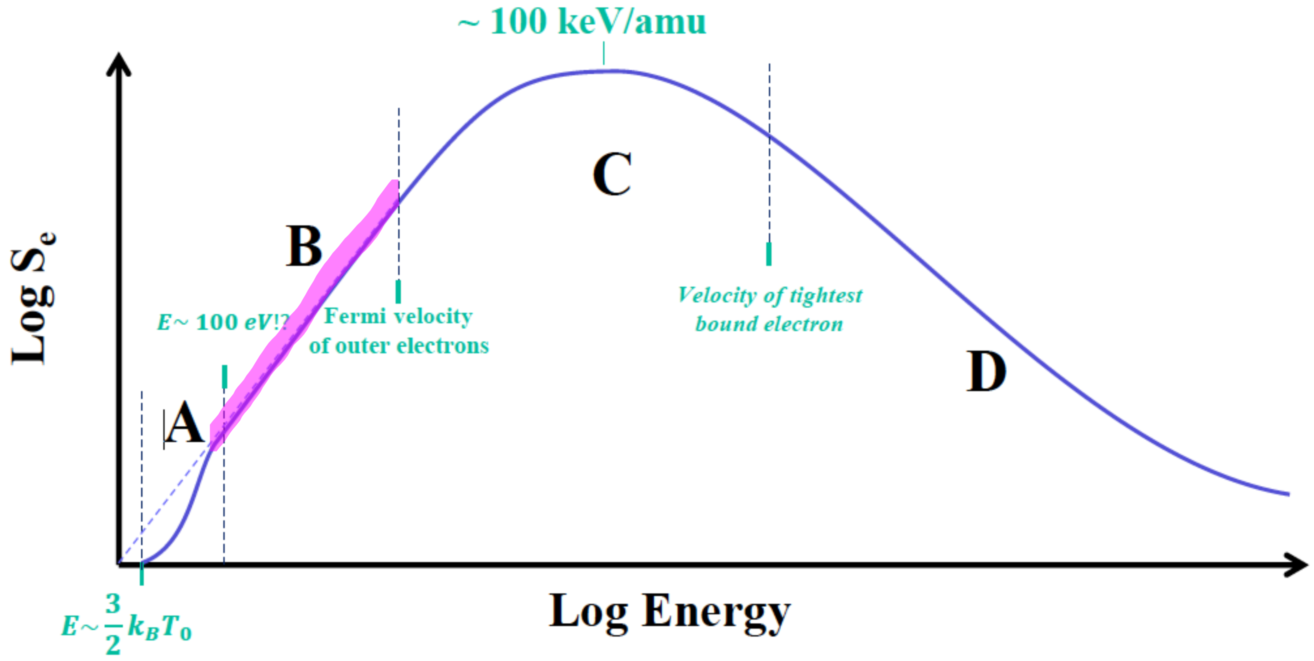
Regime A: low energy regim





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

Regime B: LSS theory

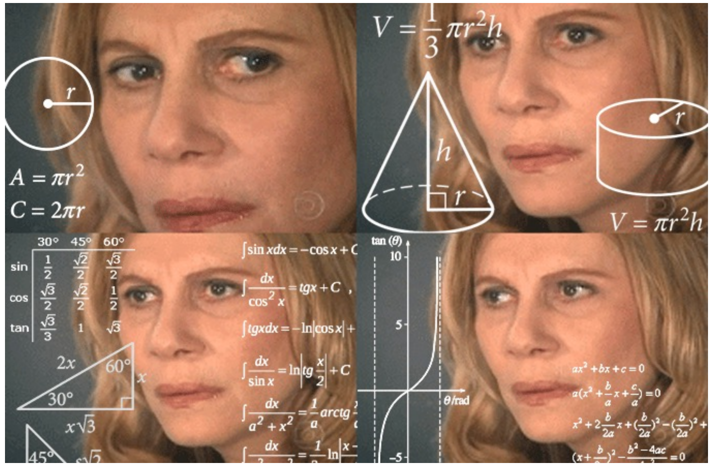


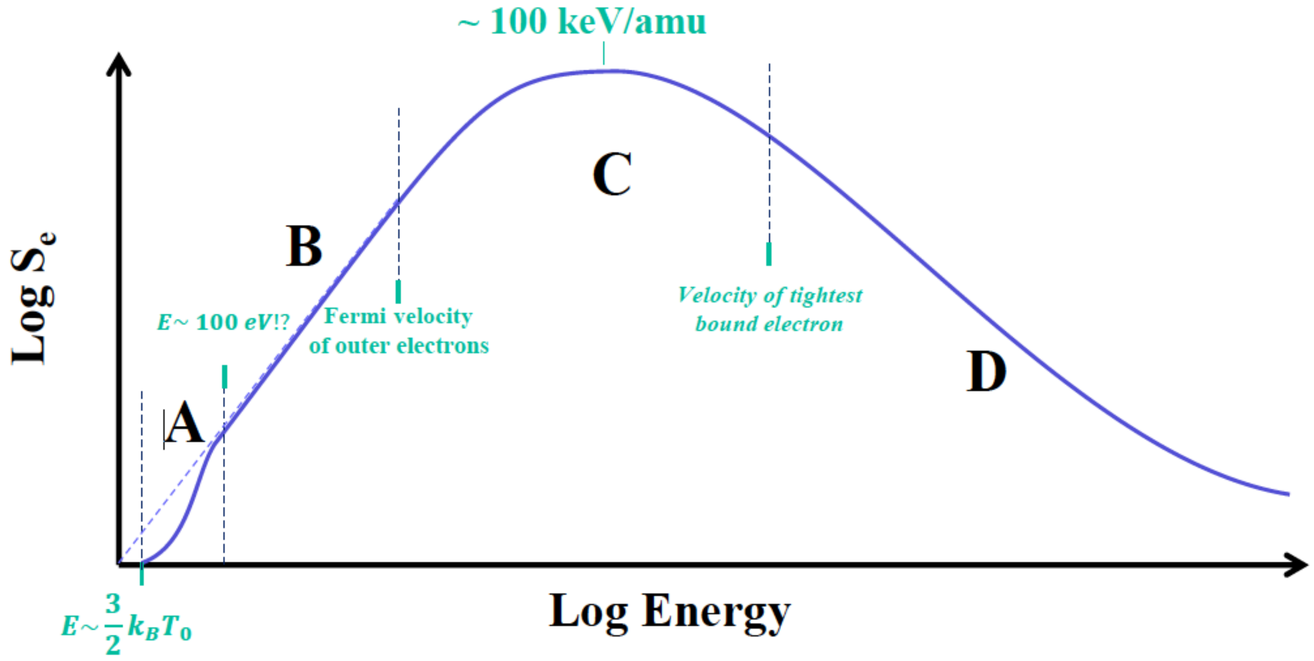
- At higher energies than region A the stopping is almost perfectly linear to the ion velocity,

  $S_e \propto v$

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

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

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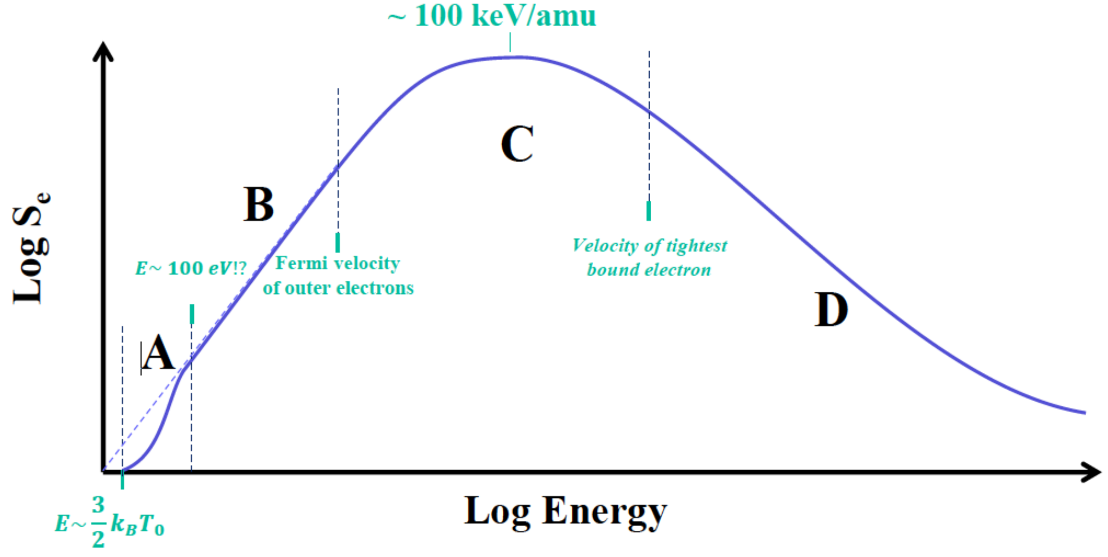
Regimes of D: Bethe-Bloch



- 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

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

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