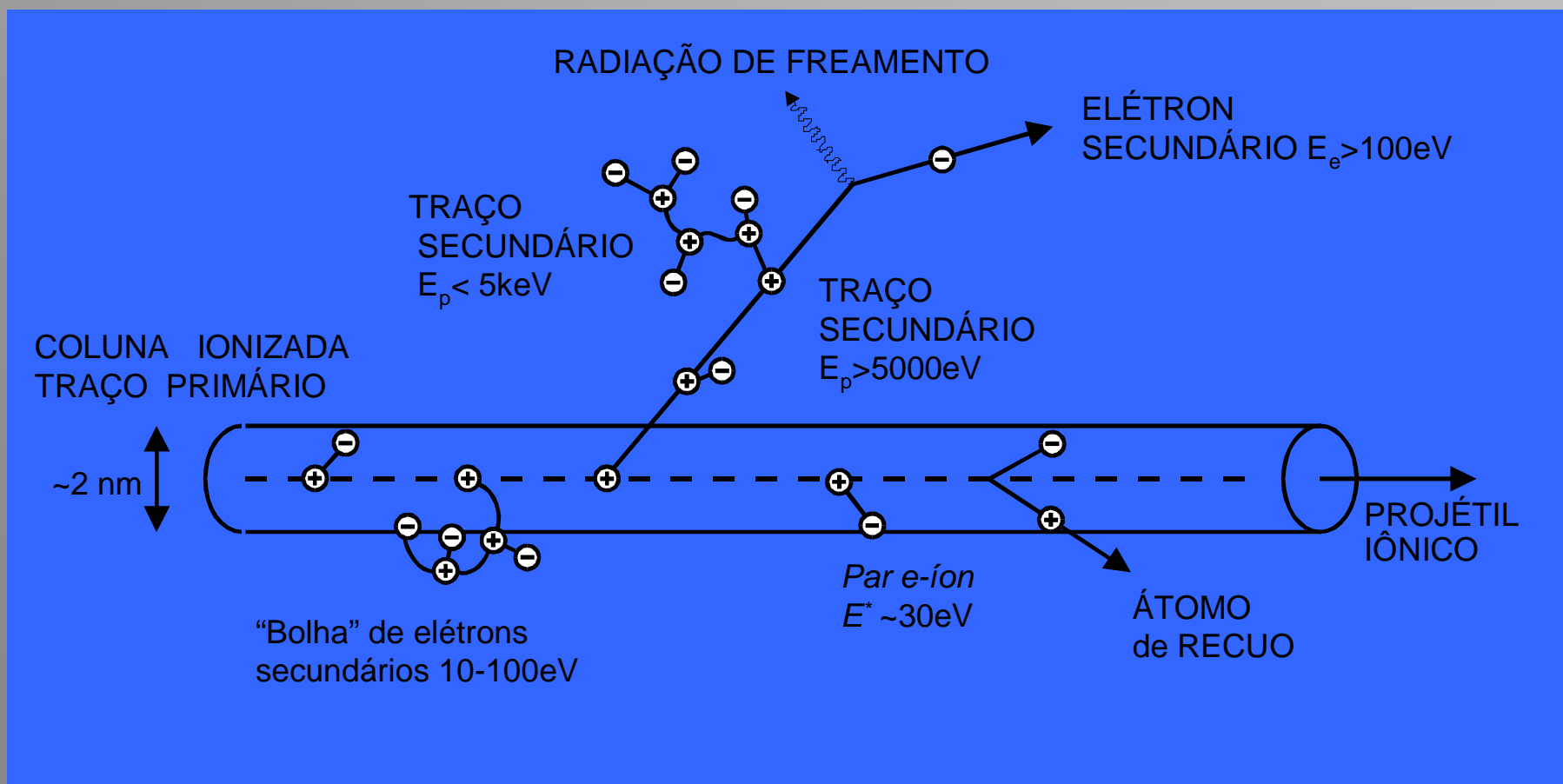


Universidade de São Paulo
Instituto de Física

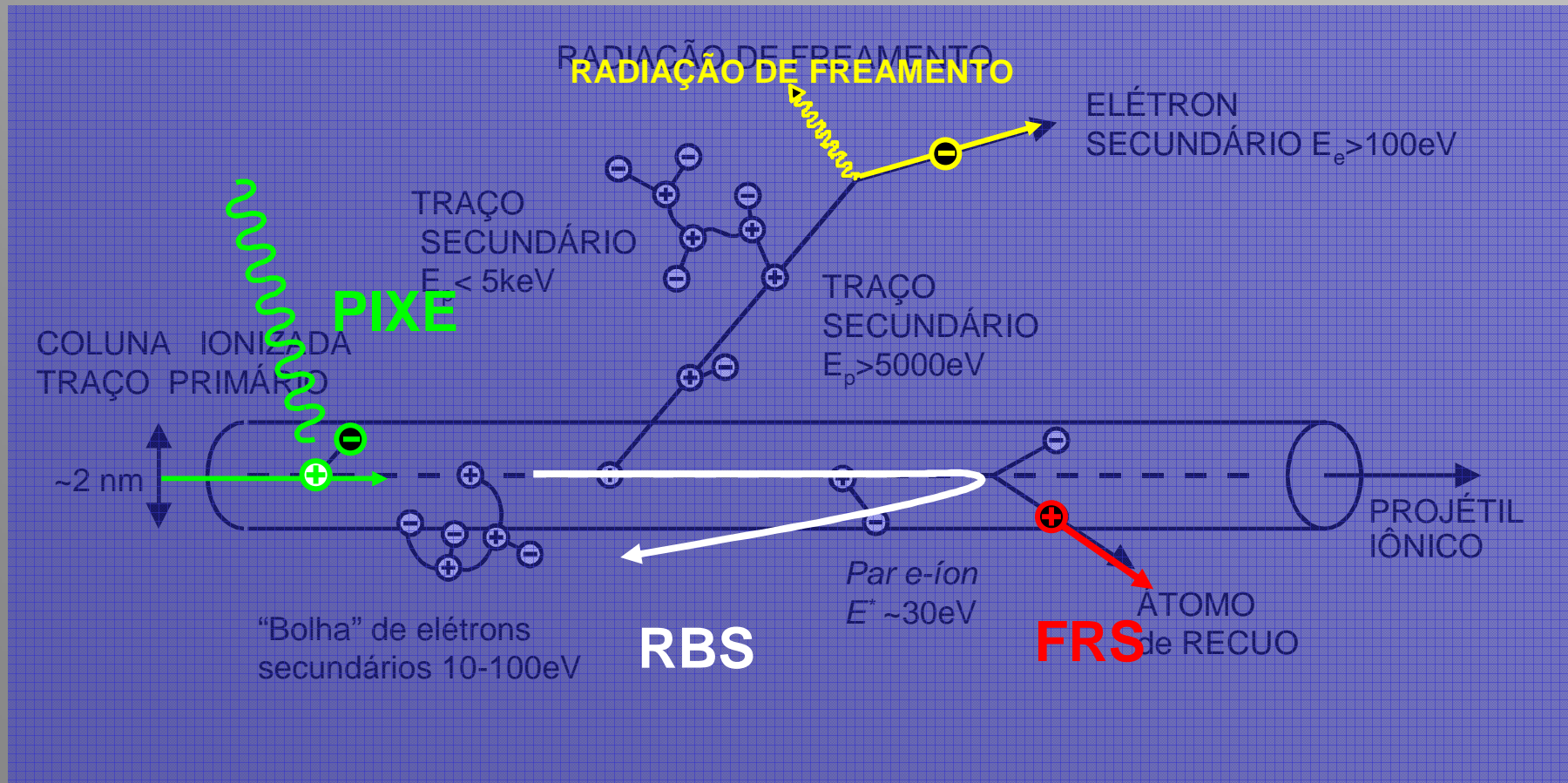
FAP5844 - Técnicas de Raios-X e de feixe iônico
aplicados à análise de materiais

Manfredo H. Tabacniks
FI4 - 2008

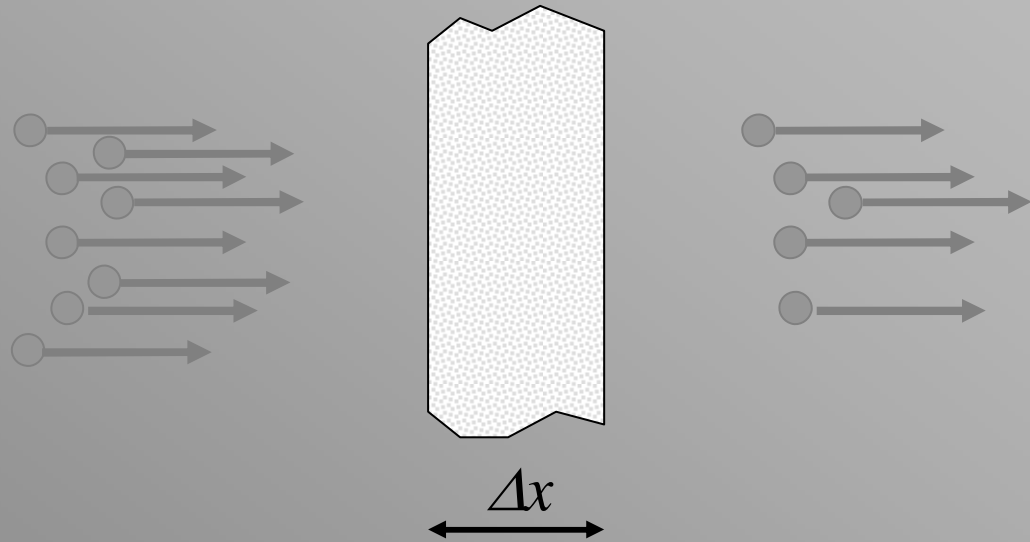
Principais processos de freamento de íons na matéria...



... e seu uso na análise de materiais



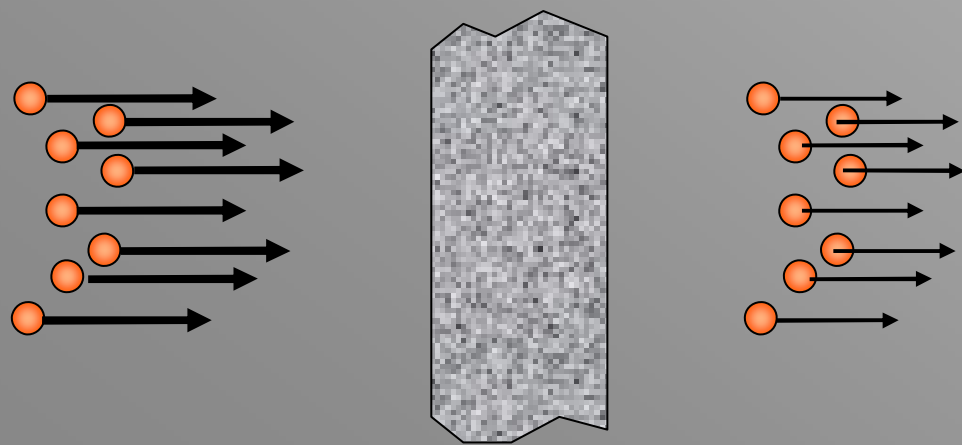
Feixe de fótons na matéria



$$\frac{N}{N_0} = e^{-\mu \cdot \Delta x}$$

$$E_v = cte$$

Feixe de íons na matéria



$$N_0 = cte$$

$$E' = E_0 - \left(\frac{dE}{dx} \right) \Delta x$$

RBS- Principais processos físicos

- Fator de Freamento
- Fator Cinemático
- Seção de Choque
- *Stragling*

Poder de freamento (*stopping power*)

$$S = -\frac{dE}{dx} \quad \left[\frac{\text{eV}}{\text{\AA}} \right]$$

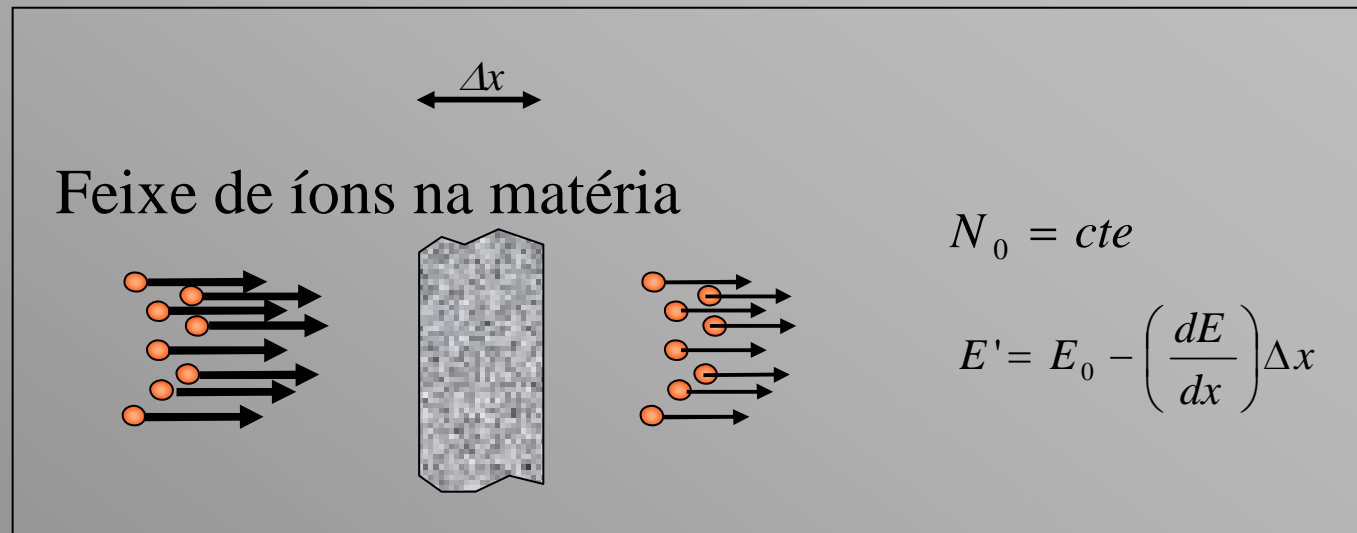
$$s = -\frac{1}{\rho} \frac{dE}{dx} \quad \left[\frac{\text{eV}}{\mu\text{g/cm}^2} \right]$$

ρ é a densidade
de massa do meio

$$\varepsilon = -\frac{1}{N} \frac{dE}{dx} \quad \left[\frac{\text{eV}}{\text{at/cm}^2} \right] = \left[\text{eVcm}^2 \right]$$

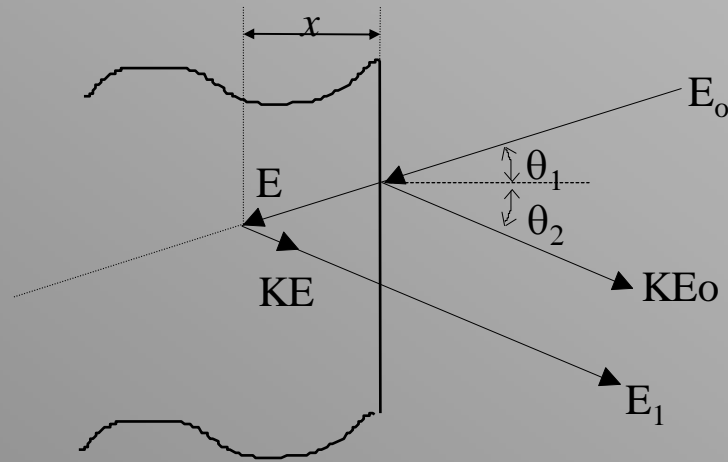
N é a densidade atômica
total do meio

Aproximação de superfície



$$\Delta E(t) = \int^{\Delta x} \frac{dE}{dx} dx \cong \left. \frac{dE}{dx} \right|_{in} \cdot \Delta x$$

fator de freamento (aproximação de superfície)



$$\Delta E_d = KE_o - E_1 = [S] \cdot x$$

relação linear entre ΔE e x

$$[S] = - \left[\frac{K}{\cos \theta_1} \frac{dE}{dx} \Big|_e + \frac{1}{\cos \theta_2} \frac{dE}{dx} \Big|_s \right]$$

$$E = E_o - \frac{x}{\cos \theta_1} \frac{dE}{dx} \Big|_e$$

$$E_1 = KE - \frac{x}{\cos \theta_2} \frac{dE}{dx} \Big|_s$$

$$S = - \frac{dE}{dx} \quad \varepsilon = - \frac{1}{N} \frac{dE}{dx}$$

fator de poder de freamento

$$[S] = \left[\frac{K S(E_o)}{\cos \theta_1} + \frac{S(KE_o)}{\cos \theta_2} \right]$$

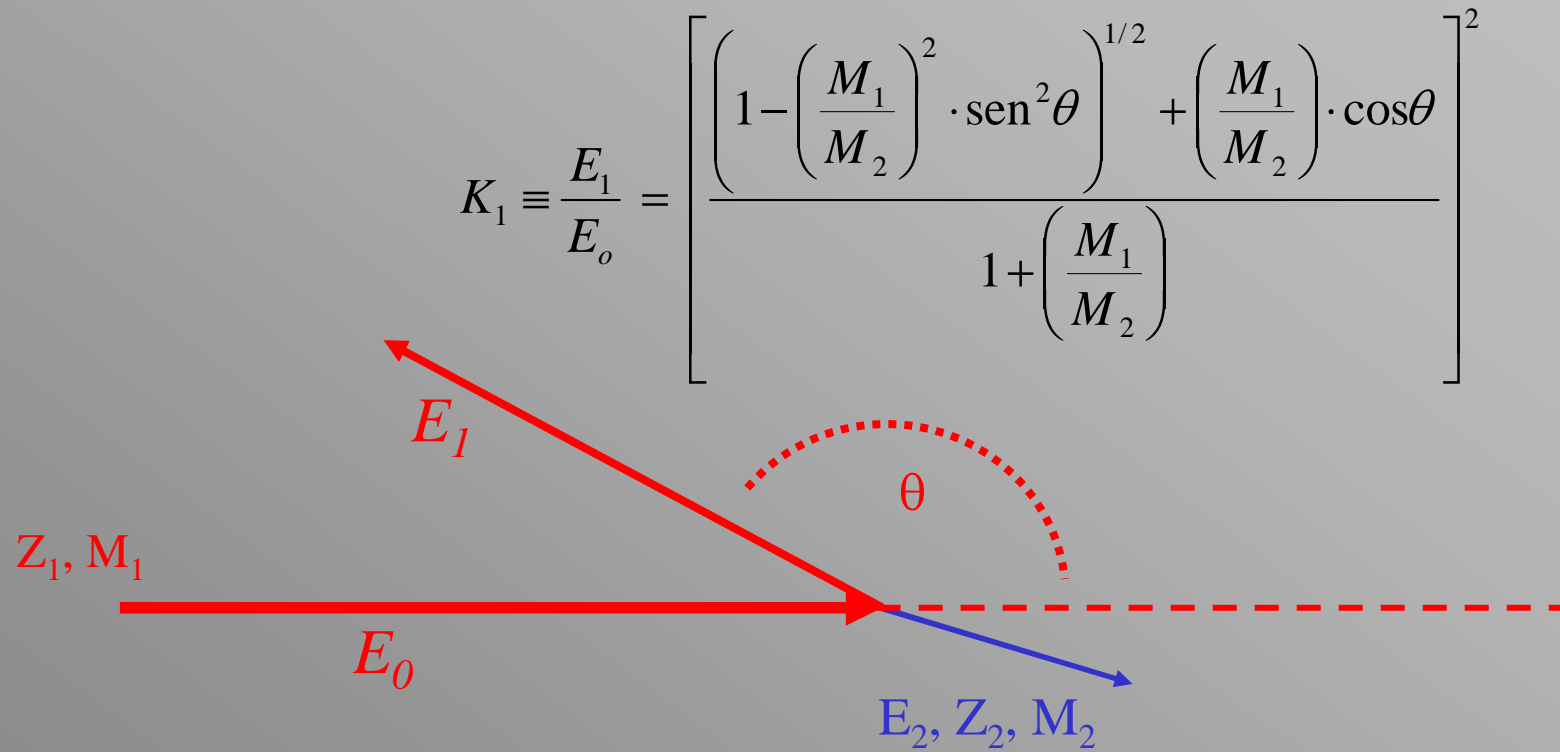
fator de seção de choque de freamento

$$[\varepsilon] = \left[\frac{K \varepsilon(E_o)}{\cos \theta_1} + \frac{\varepsilon(KE_o)}{\cos \theta_2} \right]$$

Regra de Bragg (fator de freamento para compostos)

$$\varepsilon(A_m B_n) = m\varepsilon(A) + n\varepsilon(B)$$

Fator Cinemático: Espalhamento elástico



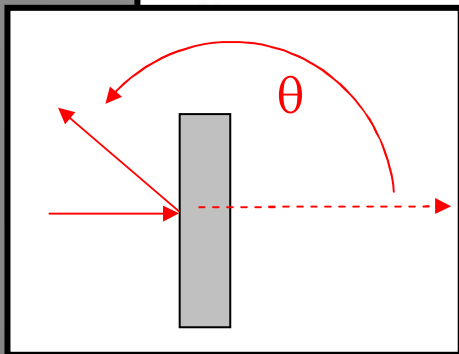
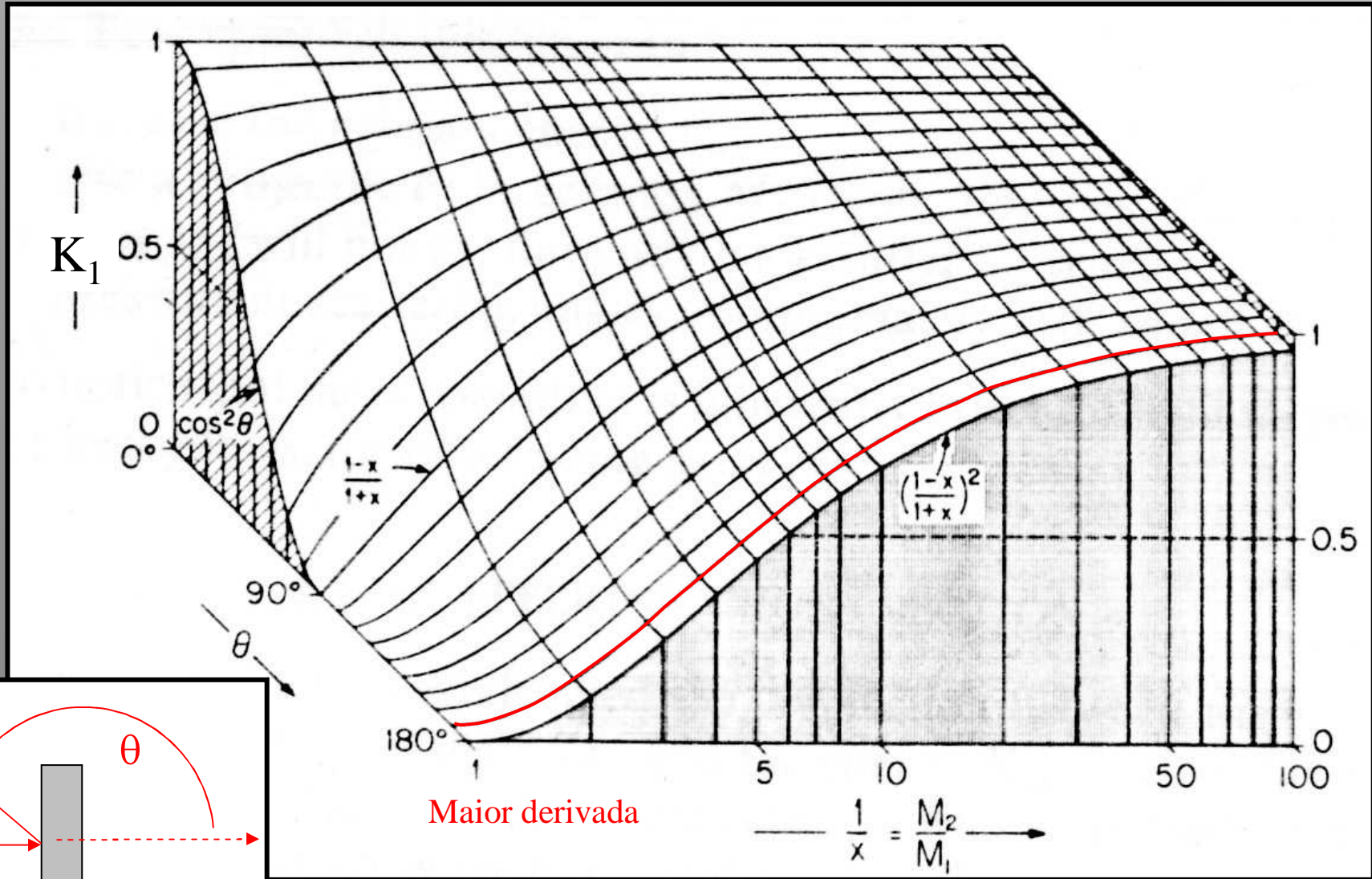
Espalhamento “head on”

$$K_M^{180} = \left[\frac{M_2 - M_1}{M_2 + M_1} \right]^2 = \left[\frac{1 - x}{1 + x} \right]^2$$

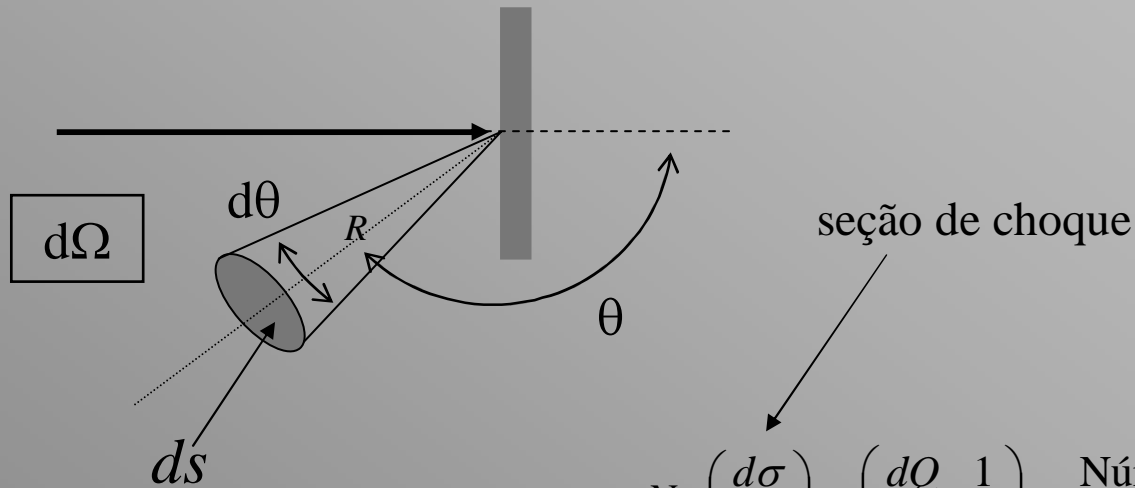
$$E_2^{180} = E_o - E_1^{180} = E_o \left[\frac{4M_1 M_2}{(M_1 + M_2)^2} \right]$$

Fator Cinemático

$$K_1 \equiv \frac{E_1}{E_o} = \left[\frac{\left(1 - \left(\frac{M_1}{M_2}\right)^2 \cdot \text{sen}^2 \theta\right)^{1/2} + \left(\frac{M_1}{M_2}\right) \cdot \text{cos} \theta}{1 + \left(\frac{M_1}{M_2}\right)} \right]^2$$



Seção de choque de espalhamento



$$N.t. \left(\frac{d\sigma}{d\Omega} \right) = \left(\frac{dQ}{d\Omega} \cdot \frac{1}{Q} \right) = \frac{\text{Número de partículas espalhadas em } d\Omega}{\text{Número total de partículas incidentes}}$$

$$d\Omega = \frac{ds}{4\pi R^2}$$

$$\frac{d\sigma}{d\Omega} = \frac{\left(\frac{\text{numero de partículas detectadas em } d\Omega}{\text{numero total de partículas incidentes}} \right)}{d\Omega.t.N} = \frac{A}{\frac{Q}{e} \cdot d\Omega.t.N}$$

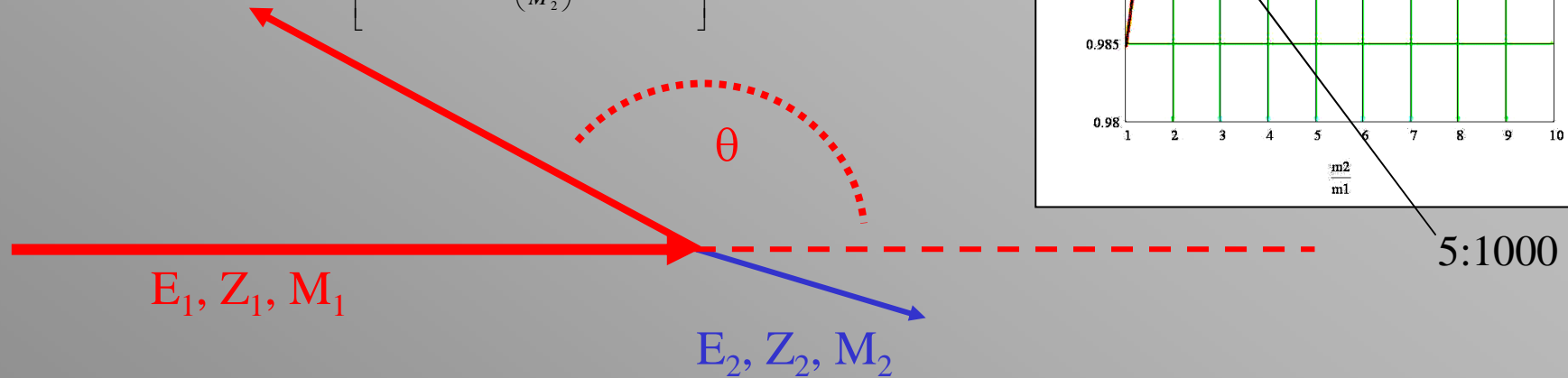
→ área do pico
→ átomos/cm²

$$\sigma = \frac{1}{\Omega} \int_{\Omega} \frac{d\sigma}{d\Omega} \cdot d\Omega$$

$$\boxed{A = \sigma \cdot \Omega \cdot Q \cdot N \cdot t}$$

Seção de choque de espalhamento Rutherford

$$K_1 \equiv \frac{E_1}{E_o} = \left[\frac{\left(1 - \left(\frac{M_1}{M_2} \right)^2 \cdot \text{sen}^2 \theta \right)^{1/2} + \left(\frac{M_1}{M_2} \right) \cdot \text{cos} \theta}{1 + \left(\frac{M_1}{M_2} \right)} \right]^2$$



Seção de choque no CM

$$\frac{d\sigma}{d\Omega}(E, \theta) = \left(\frac{Z_1 \cdot Z_2 \cdot e^2}{4 \cdot E_c} \right)^2 \frac{1}{\text{sen}^4(\theta/2)}$$

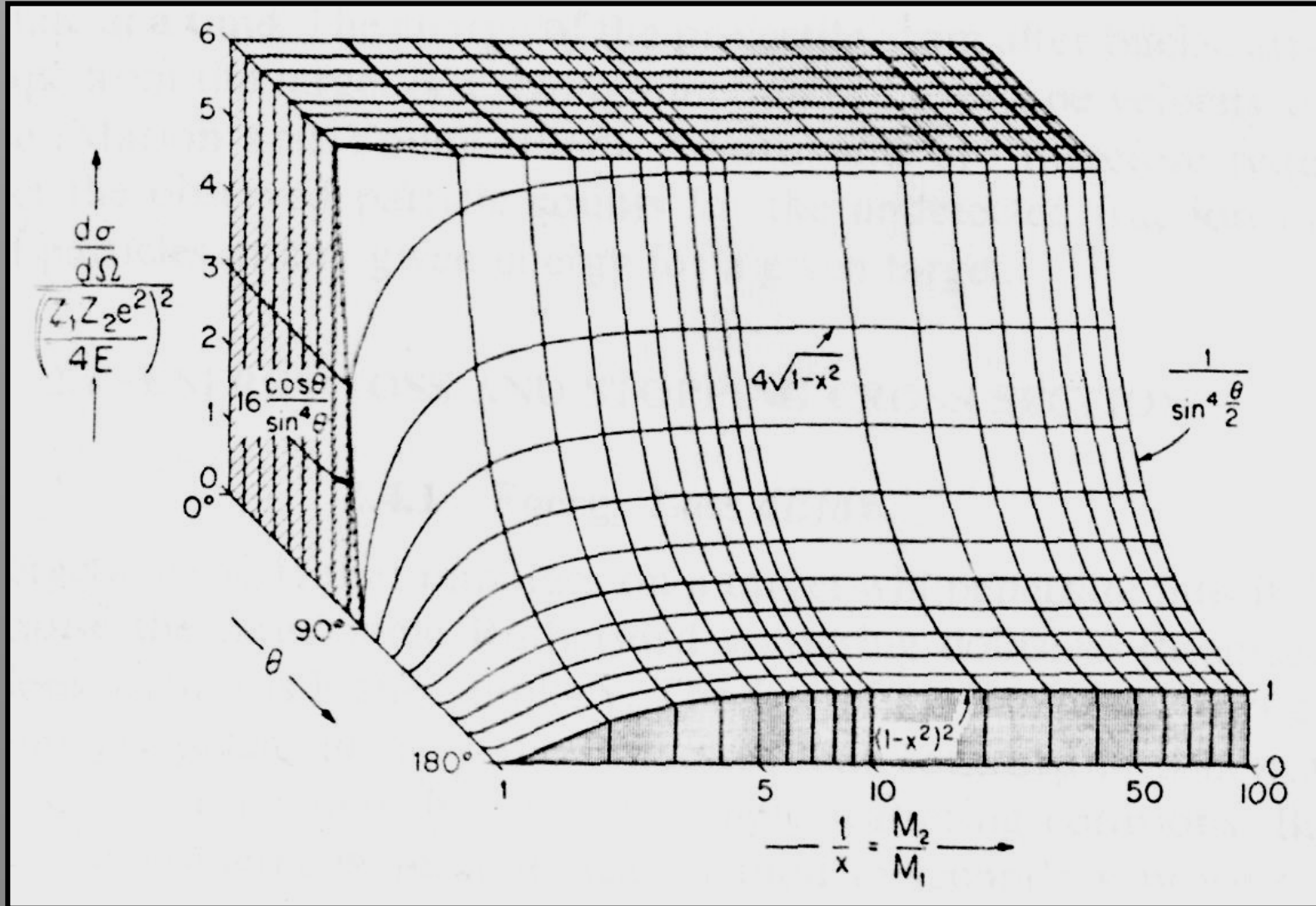
Seção de choque no laboratório

$$\frac{d\sigma}{d\Omega}(E, \theta) = \left(\frac{Z_1 \cdot Z_2 \cdot e^2}{4 \cdot E} \right)^2 \left[\frac{4}{\text{sen}^4 \theta} \frac{(a + \text{cos} \theta)^2}{a} \right]$$

$$a = \left[1 - \left(\frac{M_1}{M_2} \text{sen} \theta \right)^2 \right]^{\frac{1}{2}}$$

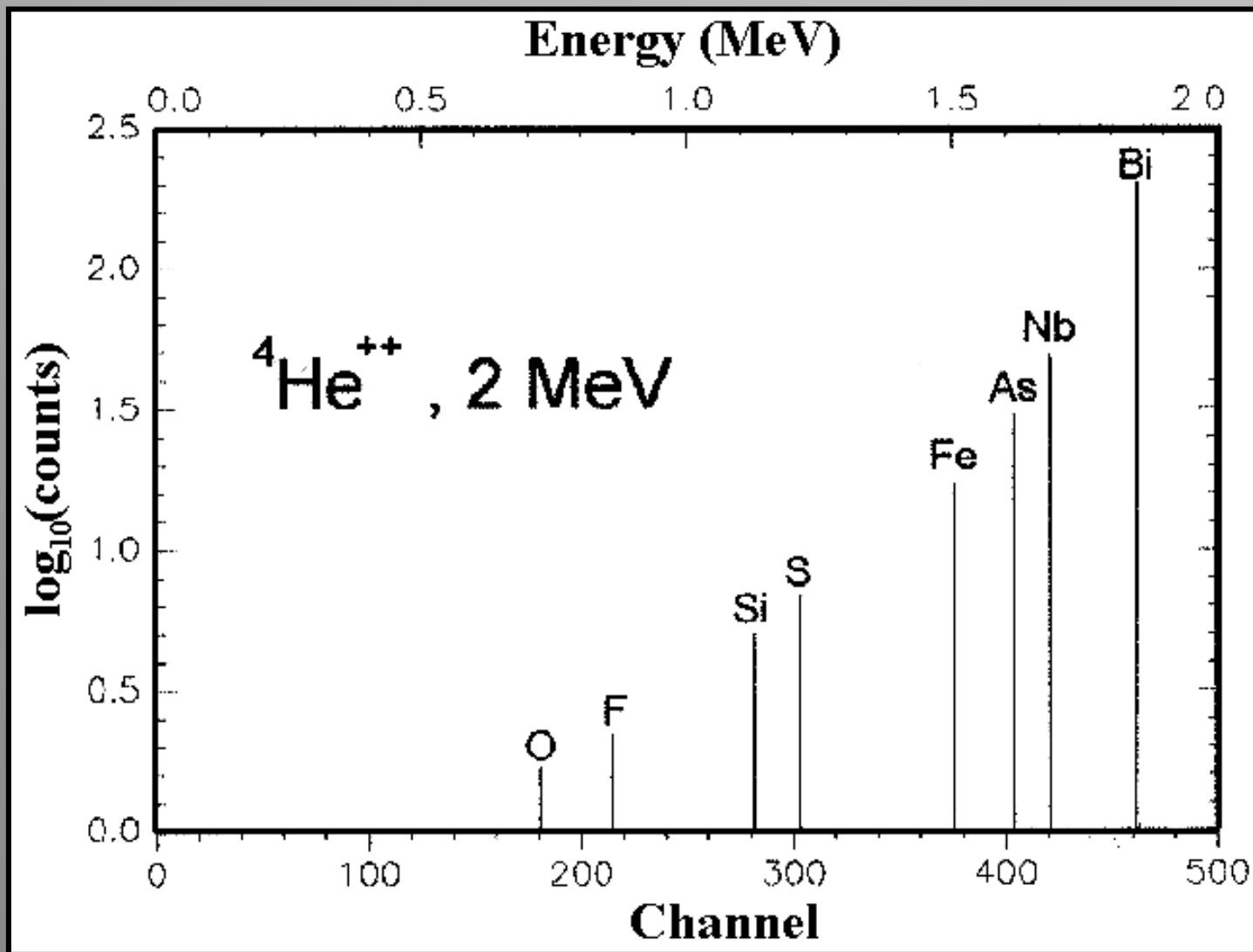
Seção de Choque

$$\frac{d\sigma}{d\Omega}(E, \theta) = \left(\frac{Z_1 \cdot Z_2 \cdot e^2}{4 \cdot E_c} \right)^2 \frac{1}{\sin^4(\theta/2)}$$



Chu, Mayer & Nicolet, 1978

Espectro de camadas monoatômicas



Z

83

41

33

26

16

14

9

8

A

16 19

28

32

56

93

209

75

Straggling

Variação quadrática média da distribuição de energia

Fórmula de Bohr $\Omega_B^2 = 4\pi Z_1^2 e^4 Z_2 N x$

espessura

densidade atômica

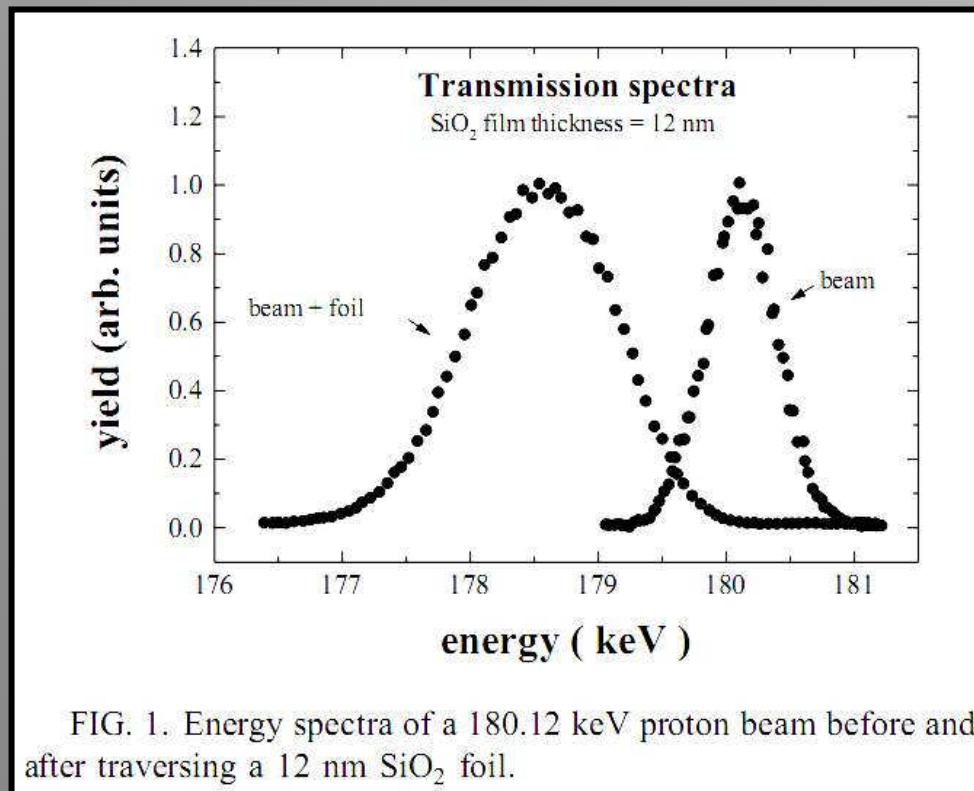
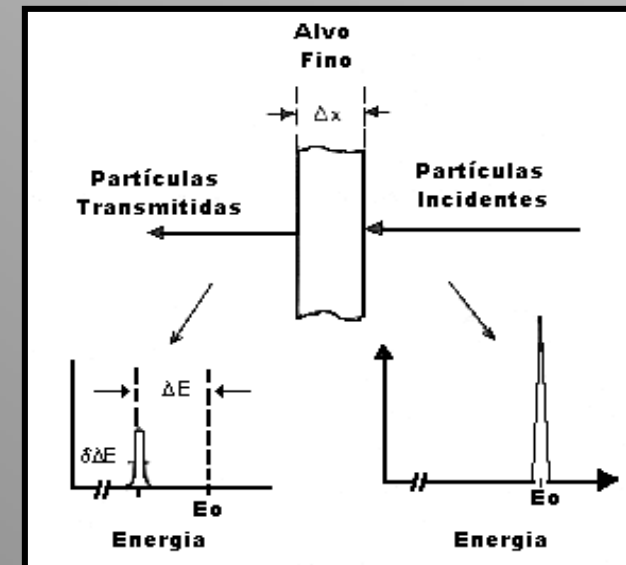
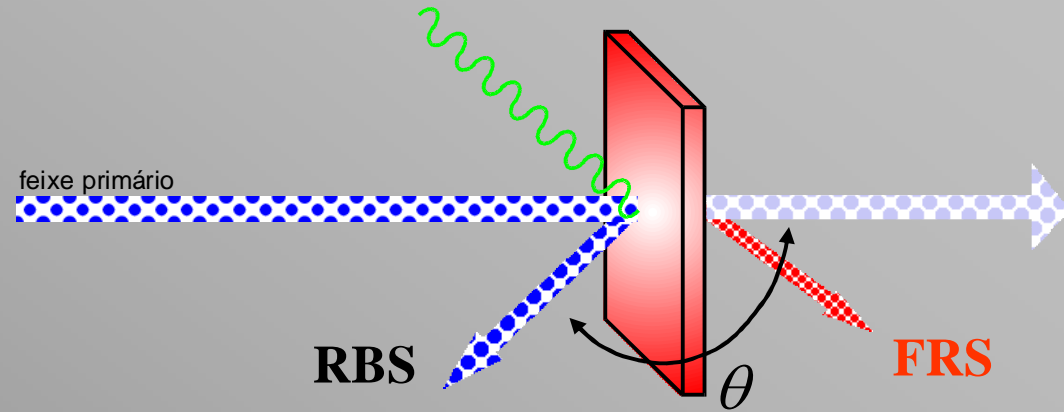
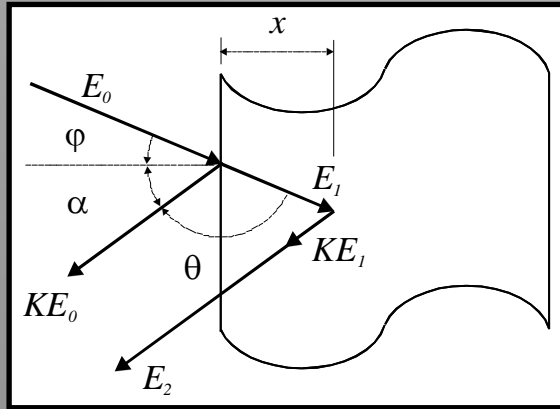


FIG. 1. Energy spectra of a 180.12 keV proton beam before and after traversing a 12 nm SiO₂ foil.

Santos et. al. Phys. Rev. A68 (2003)



RBS-FRS



Poder de Freamento

$$-\frac{dE}{dx} = \frac{4\pi Z_1^2 e^4}{mv^2} NZ_2 \ln \frac{2mv^2}{I}$$

Fator de Freamento

$$[S]_I^{meio} = \left[\frac{K_1 S(E_o)}{\cos \varphi} + \frac{S(K_1 E_o)}{\cos \alpha} \right]$$

Seção de choque Rutherford

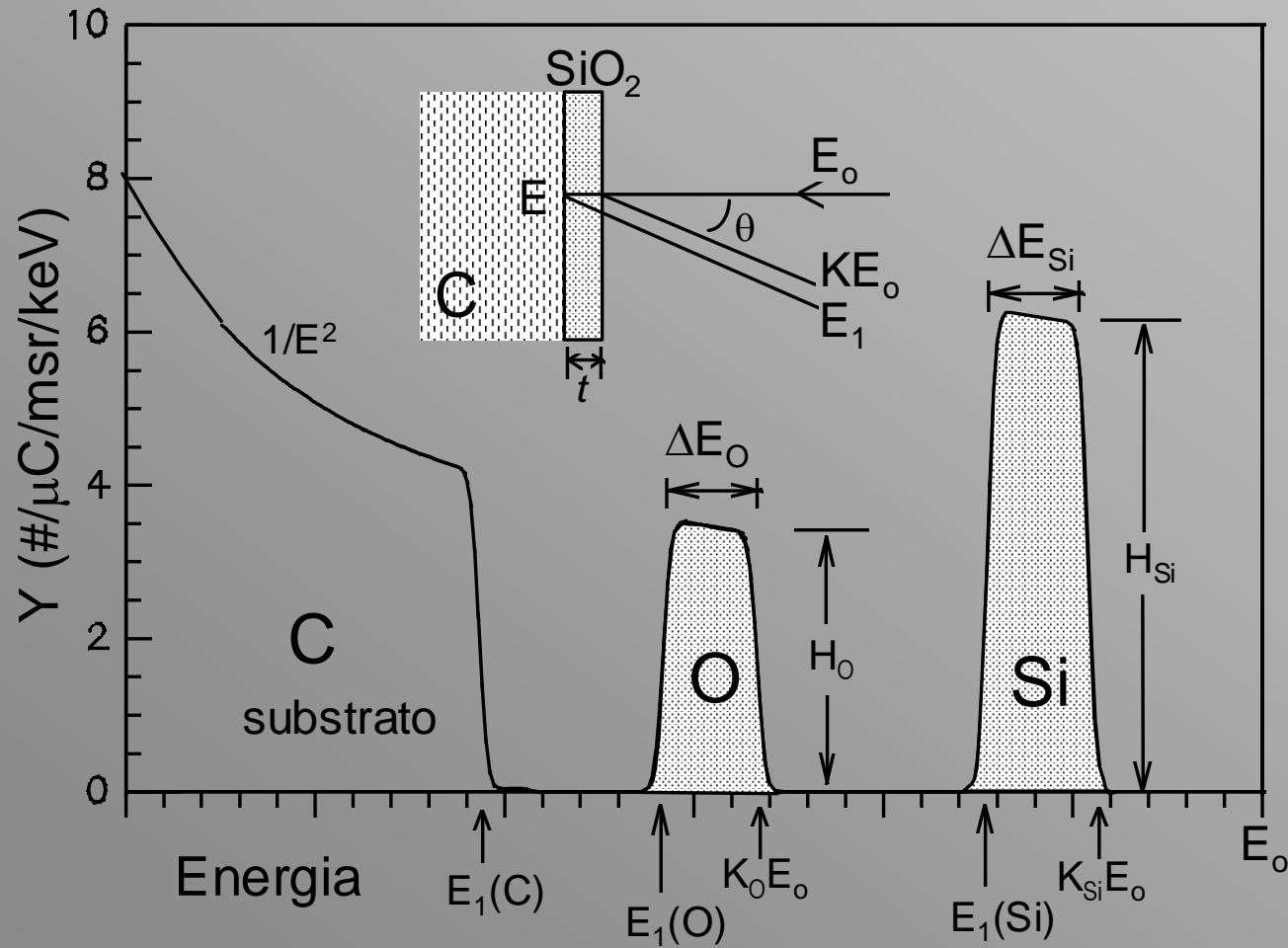
$$\frac{d\sigma}{d\Omega}(E_c, \theta_c) = \left(\frac{1}{4\pi\epsilon_0} \right)^2 \left(\frac{Z_1 \cdot Z_2 \cdot e^2}{4 \cdot E_c} \right)^2 \frac{4}{\text{sen}^4(\theta_c/2)} \left(\frac{(a + \cos \theta)^2}{a} \right)$$

$$N_i = cte \frac{\Omega}{4\pi} \cdot Q \cdot \frac{Z_1^2 Z_2^2}{E^2} \cdot \frac{\rho_i \ell}{\cos \varphi}$$

Medido

Densidade
elementar
na amostra:
átomos/cm²

RBS – Estequiometria de um composto



$$\Delta E_O = [S]_O^{meio} . t$$

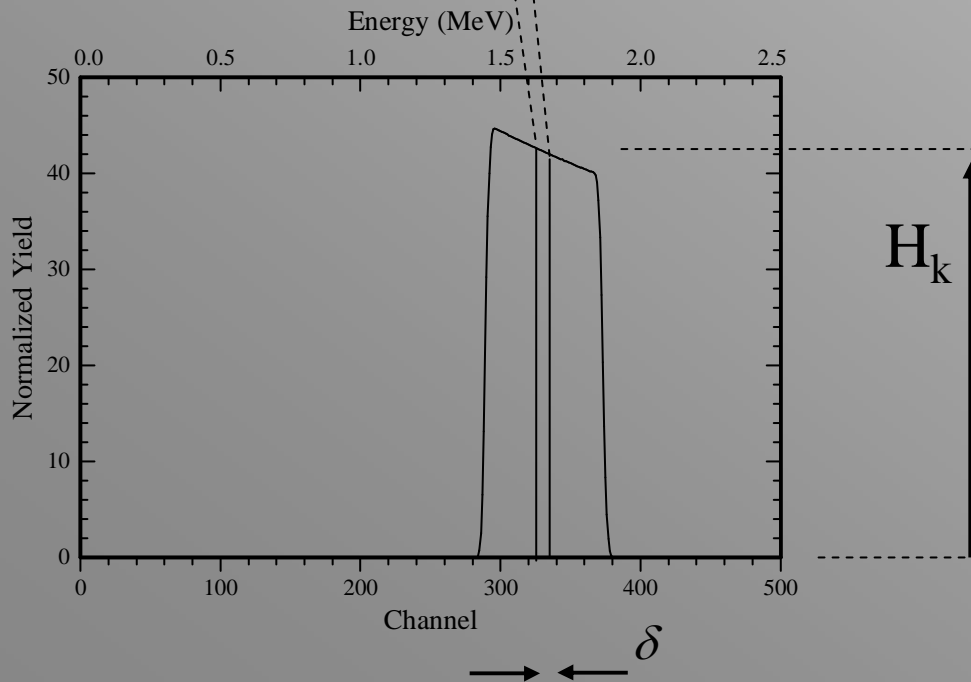
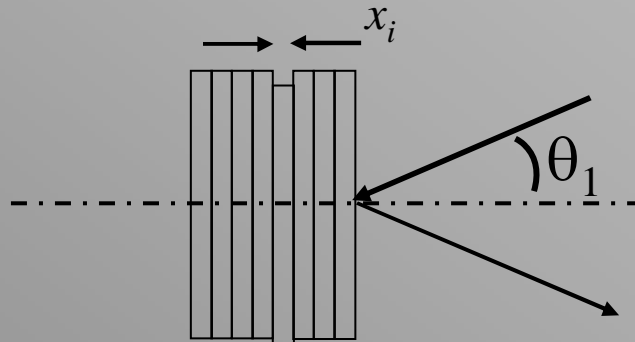
$$\Delta E_{Si} = [S]_{Si}^{meio} . t$$

$$E_I(C) = K_C E_0 - [S].t$$

$$E_I(O) = K_O E_0 - [S].t$$

$$E_I(Si) = K_{Si} E_0 - [S].t$$

Altura de picos e patamares



$$H_k = \sigma_i(E_k) \cdot \Omega \cdot Q \cdot N_i \cdot \left(\frac{x_i}{\cos \theta_1} \right)$$

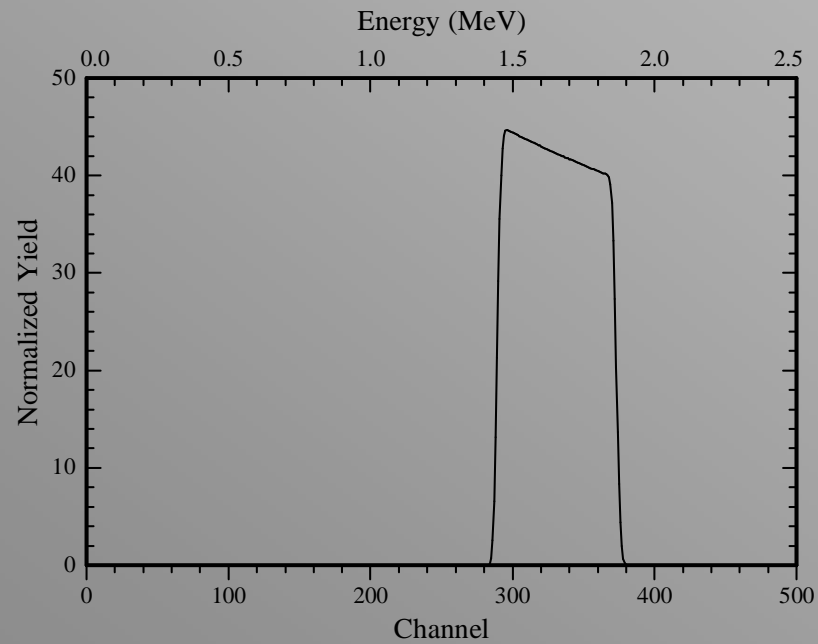
$$H_k = \sigma_i(E_k) \cdot \Omega \cdot Q \cdot n_i \cdot \left(\frac{\delta}{[\epsilon_o]_i^{meio} \cos \theta_1} \right)$$

na superfície

$$H_0 = \sigma_i(E_0) \cdot \Omega \cdot Q \cdot n_i \cdot \left(\frac{\delta}{[\epsilon_o]_i^{meio} \cos \theta_1} \right)$$

$$\frac{H_{oA}}{H_{oB}} = \frac{\sigma_A(E_o) n_A [\epsilon_o]_B^{meio}}{\sigma_B(E_o) n_B [\epsilon_o]_A^{meio}}$$

Áreas de picos



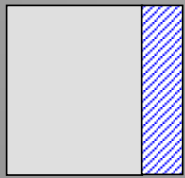
$$A_o = \sigma_i(E_o) \cdot \Omega \cdot Q \cdot N_i \cdot \left(\frac{t}{\cos \theta_1} \right)$$

$$\frac{A_{oA}}{A_{oB}} = \frac{\sigma_{iA}(E_o)}{\sigma_{iB}(E_o)} \cdot \frac{N_A}{N_B} = \left(\frac{Z_A}{Z_B} \right)^2 \frac{N_A}{N_B}$$

RBS – Contaminantes na superfície (oxidação)

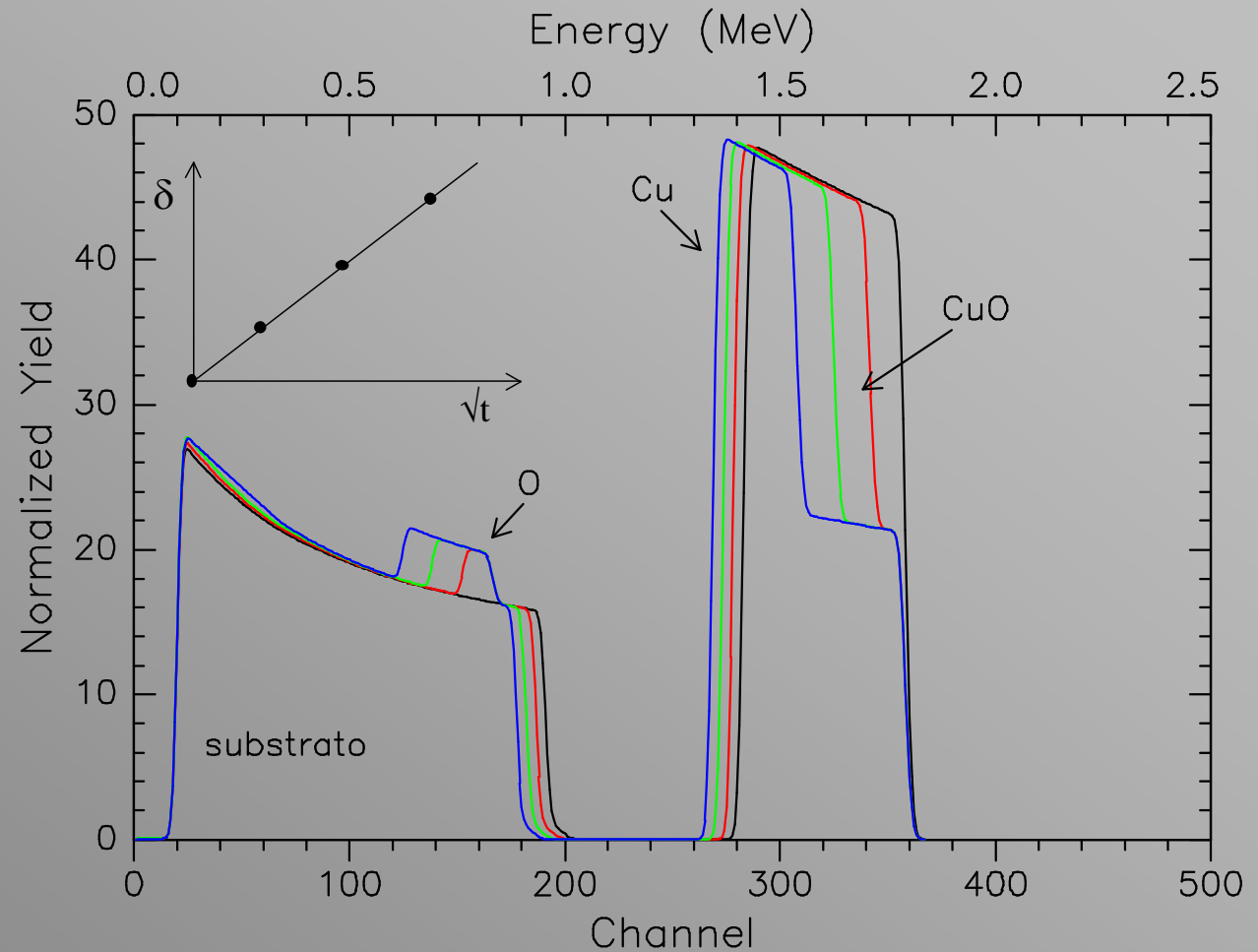
Condição Inicial

$T_{\text{Amb}}, t=0\text{s}$



Amostra Recozida

$T = 180\text{ }^{\circ}\text{C}$, $\Delta t = 2, 4, 16\text{ h}$
Atmosfera de O_2



RBS – Reações na interface de filmes finos

CONDIÇÃO INICIAL

$T_{amb}, t=0$

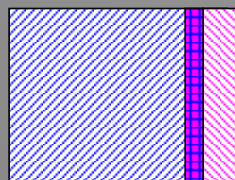


AMOSTRA RECOZIDA

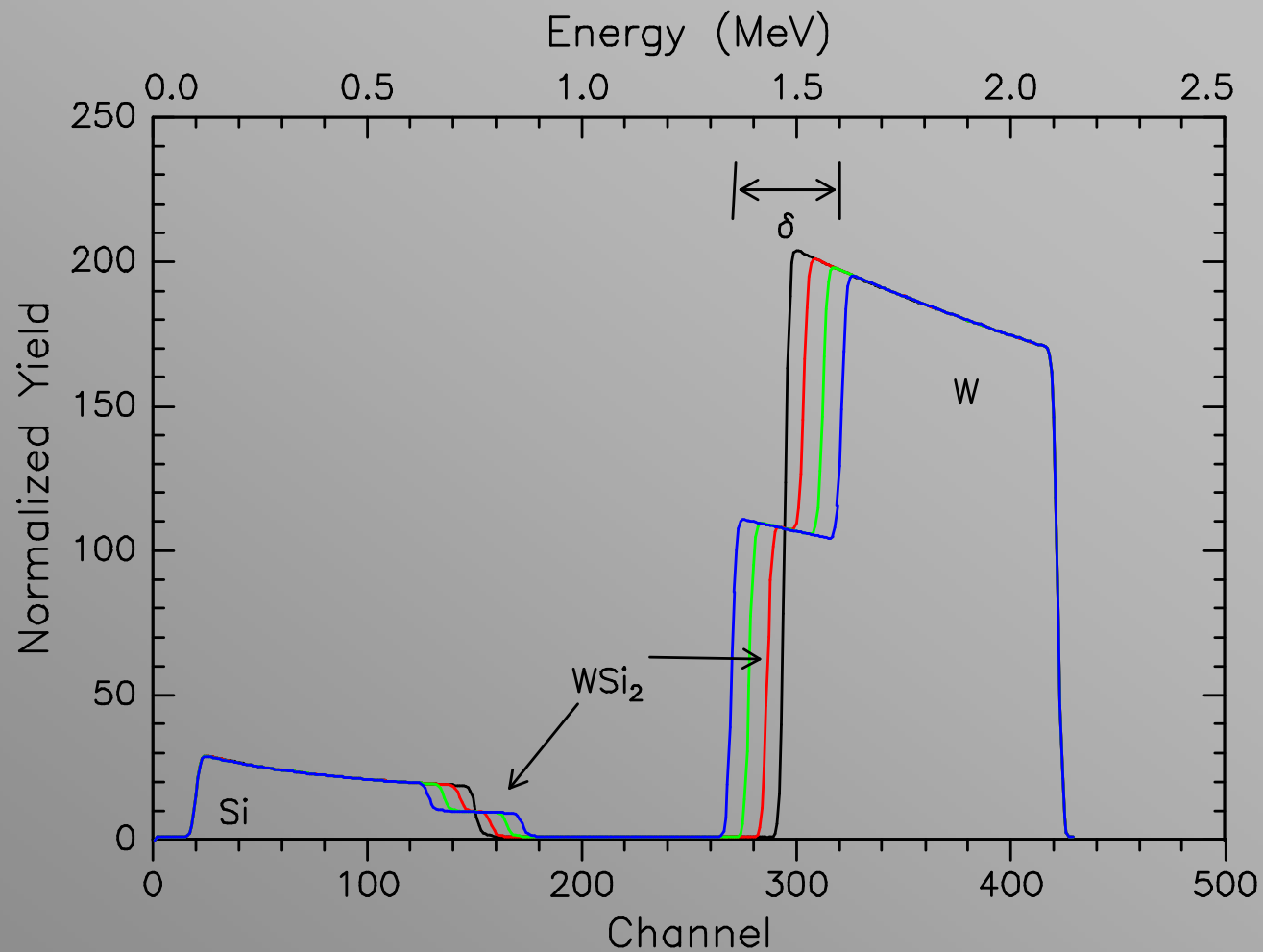
$\Delta t = 2,4,16h$

$T=500^\circ$

Atmosfera

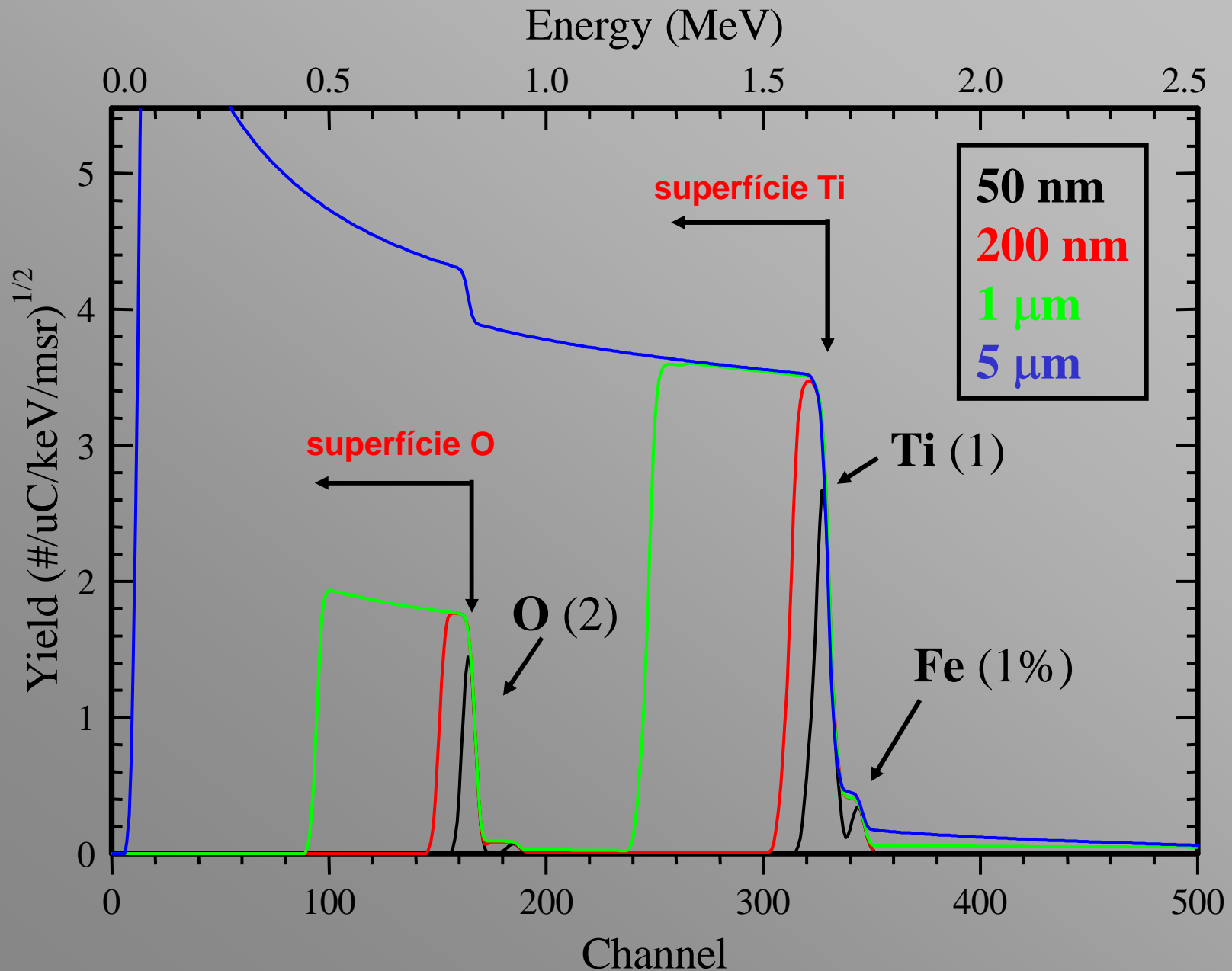


WSi_2

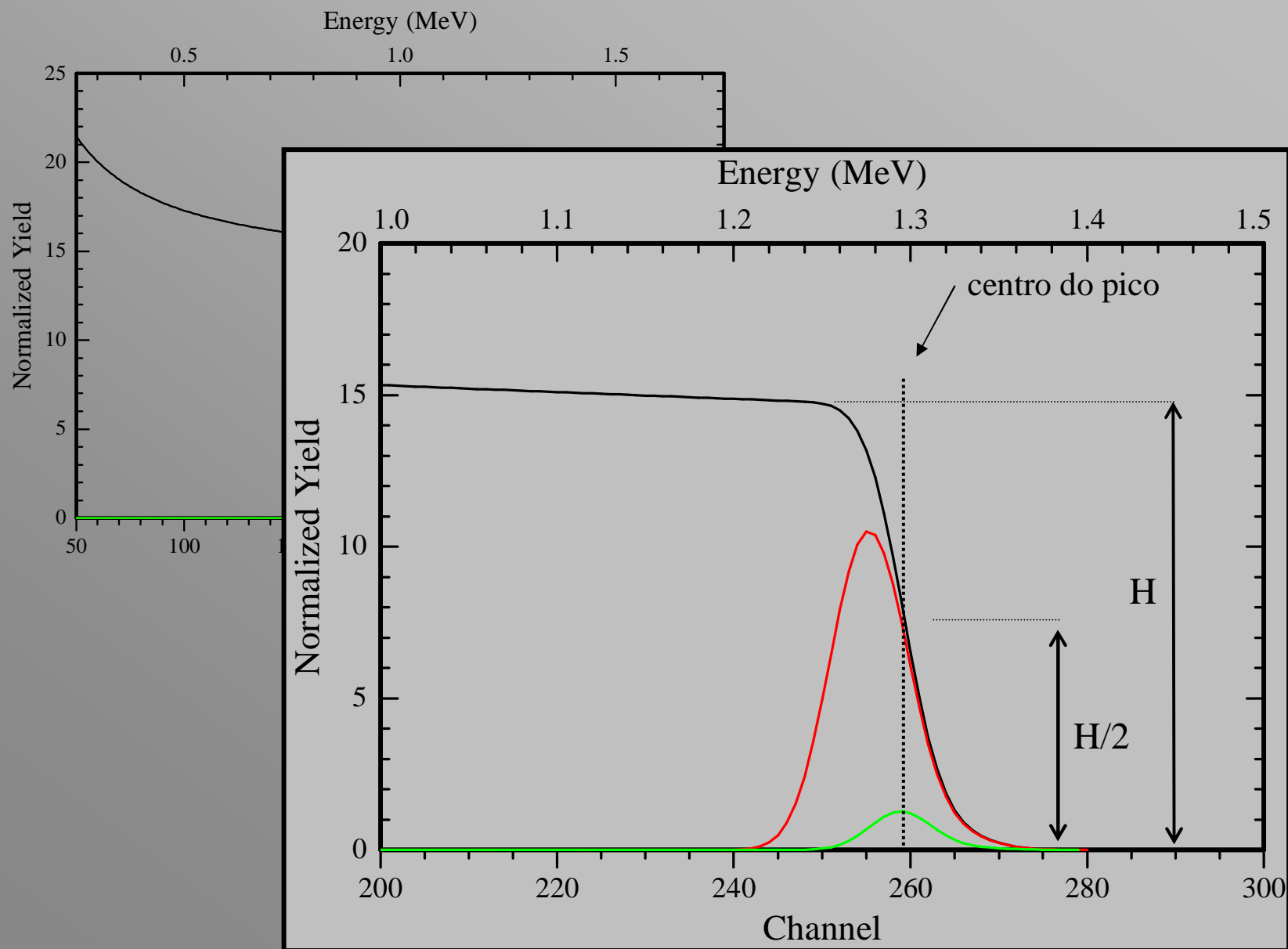


RBS para estudos de transporte de massa em filmes finos

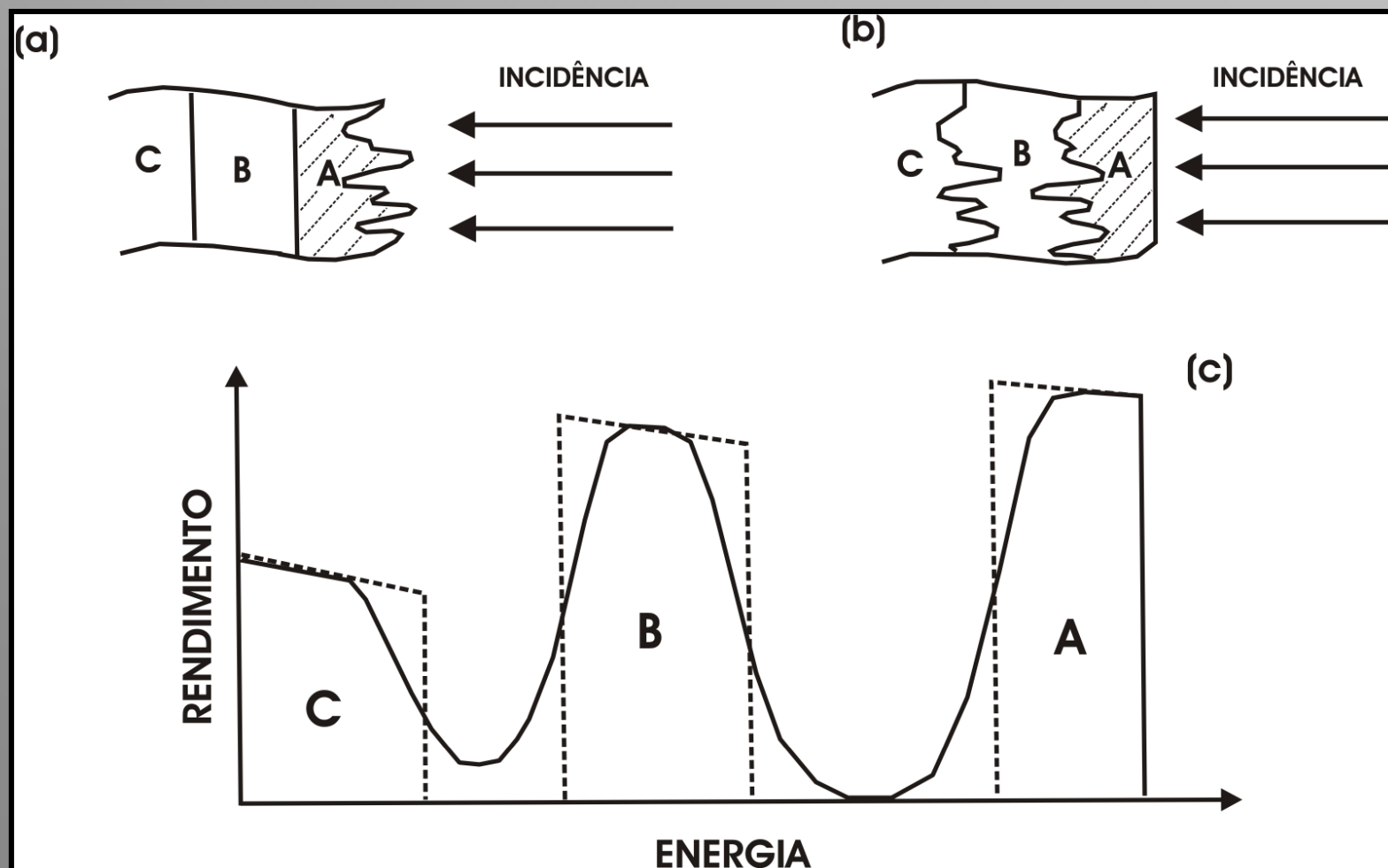
RBS - Efeito da espessura (amostra de TiO_2)



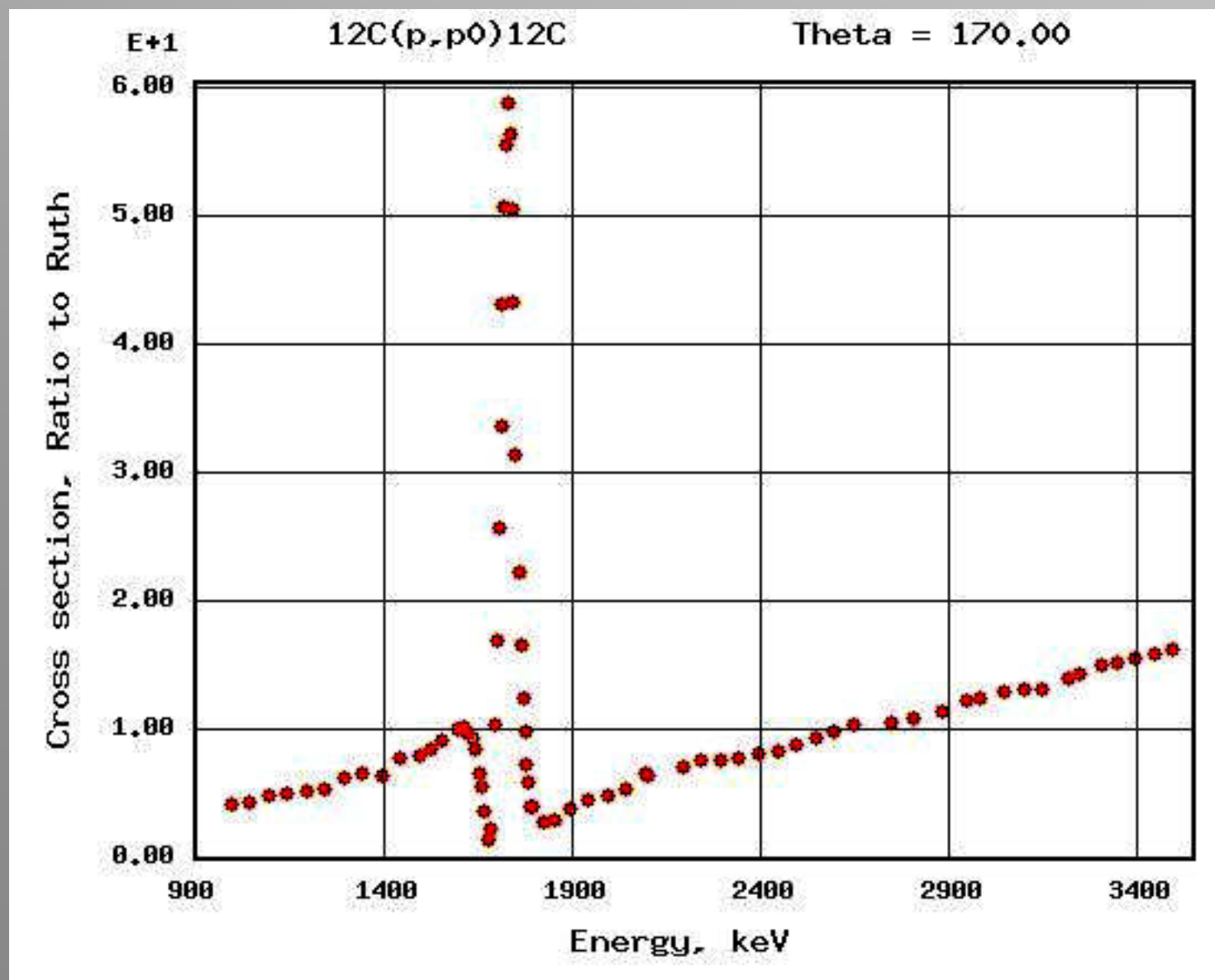
Centro de energia de um pico



Rugosidade



Ressonâncias



Ressonâncias

