Theoretical studies for energy spectra of sputtered atoms due to low-energy light ions

US-Japan Workshop on Low-Energy Ion Sputtering

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Presentation Outline

1) Motivation
   - Thompson formula

2) Derivation for a new formula
   - Low-energy light ion bombardment
   - Deviation from Thompson formula

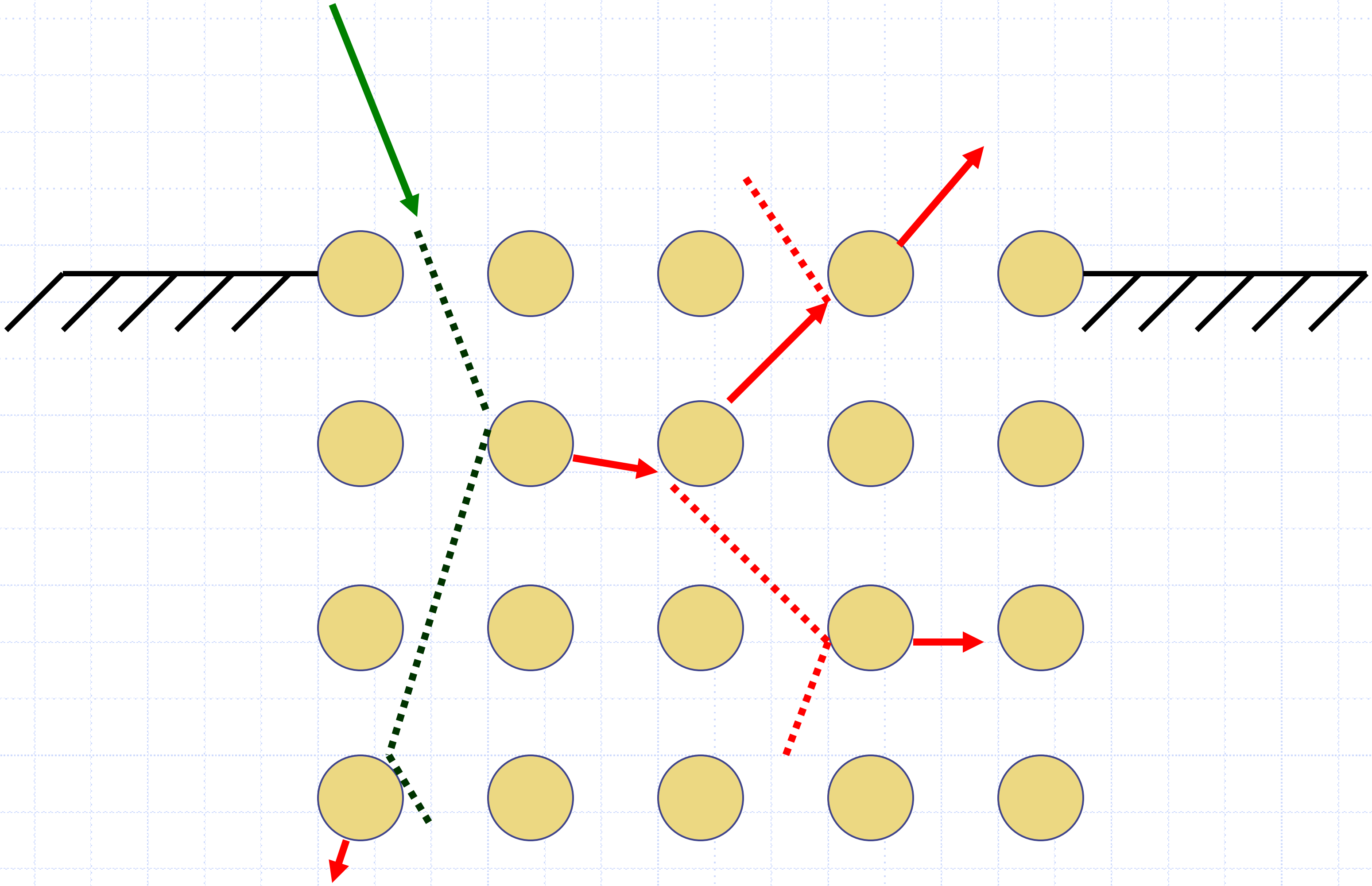
3) Highlight Data of the new formula
   - Comparison the new formula with the ACAT data

4) Summary

Motivation

- Early studies
  - Thompson formula for a linear collision cascade
- Deviation from Thompson
  - Low-energy light ion sputtering
- A new formula
  - Single knock-on cascade

Linear Collision Cascade



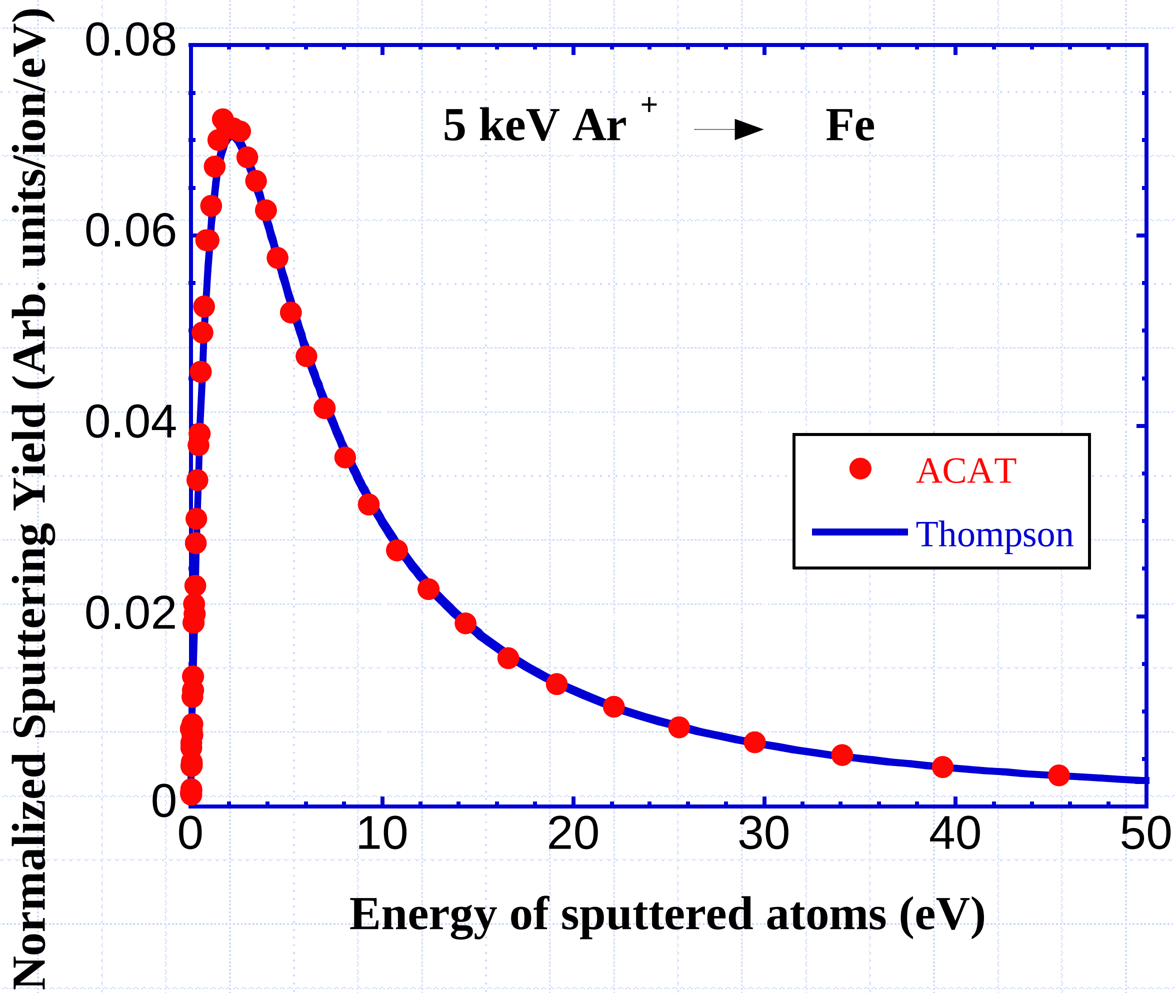
Energy spectrum due to linear collision cascade

Thompson formula

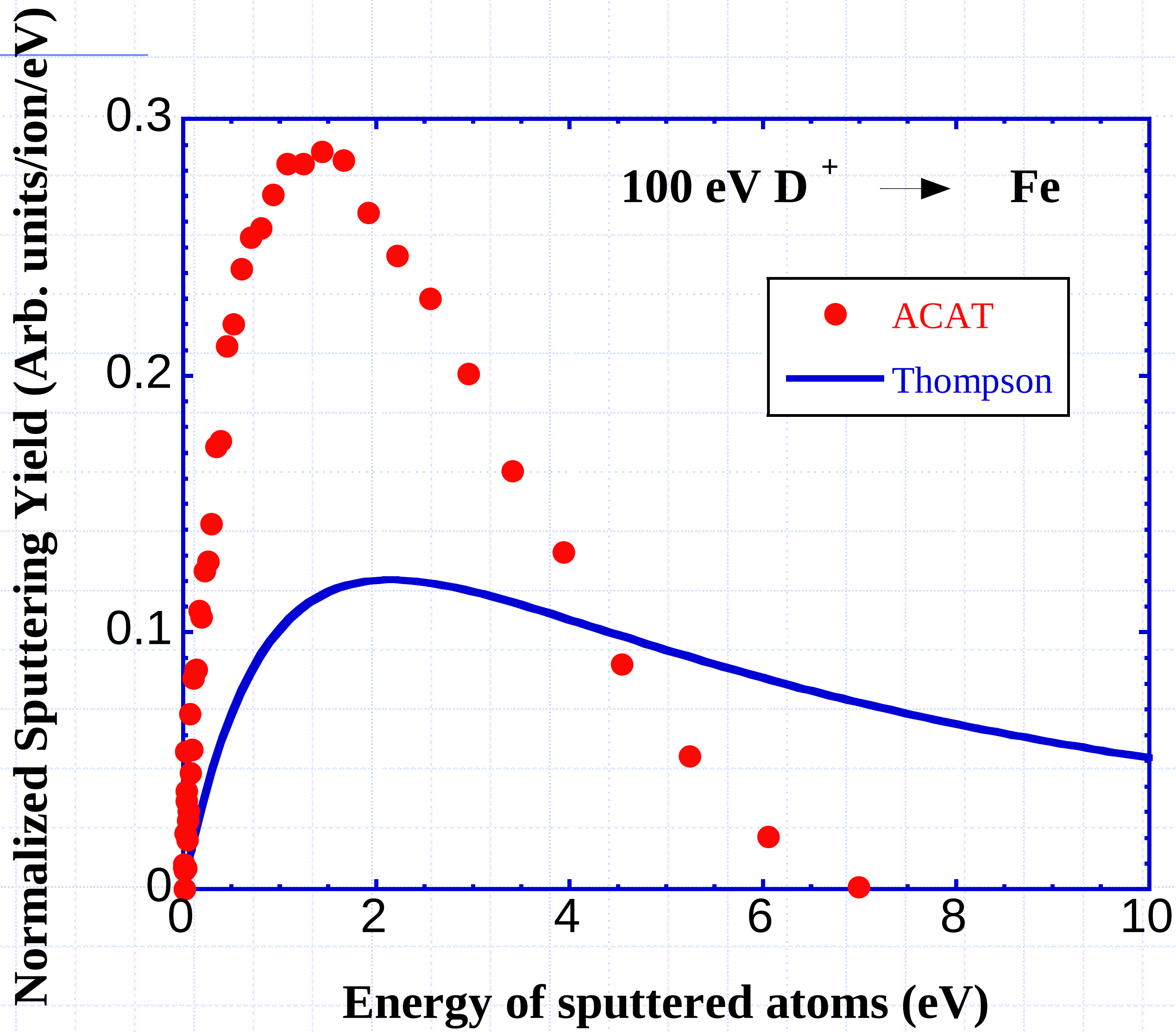
$$Y(E)dE \propto \frac{E}{(E+U_S)^3} dE$$

E : energy of sputtered atoms

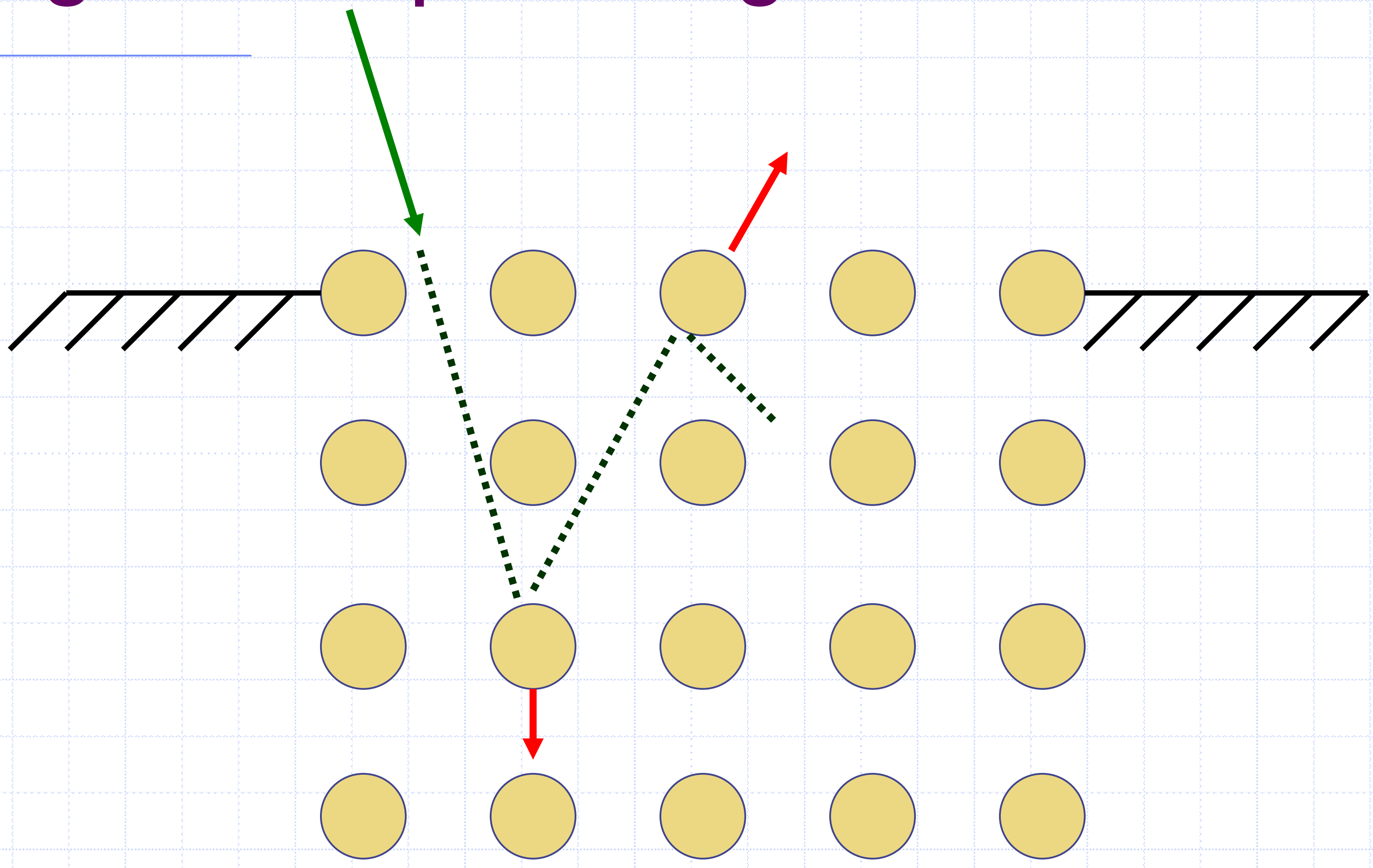
U_S : surface binding energy



Energy spectrum due to low-energy light-ions



Light-ion sputtering



single-knock-on cascade

ACAT data of sputtering

- Generation of sputtered atoms

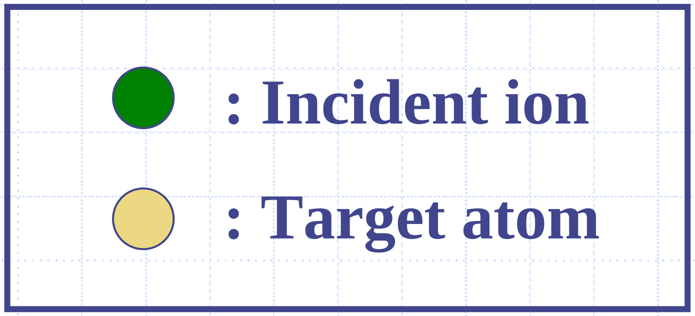
i) $D^+ \rightarrow Fe$

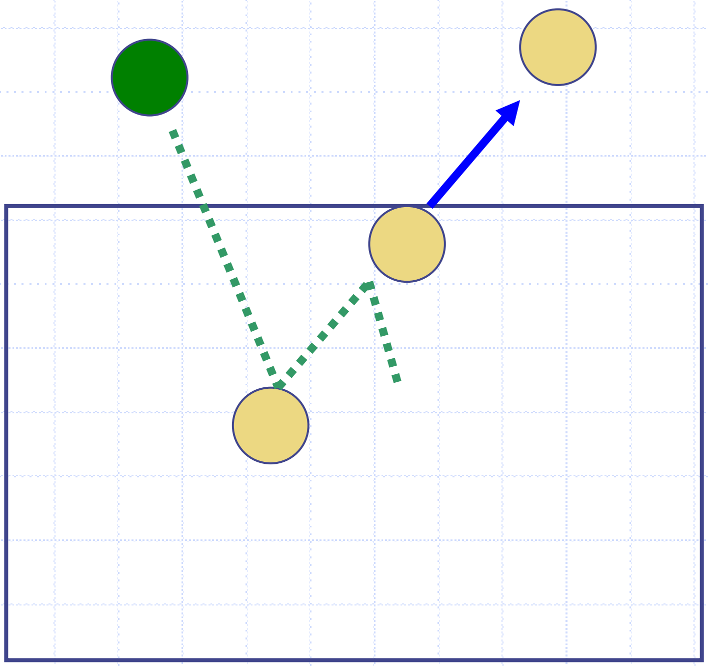
Energy \ Generation	1	2	3	4	More than 5	Average
50 eV	0.961	0.0373	0.00127	0	0	1.04
100 eV	0.776	0.187	0.0322	0.00436	5.93×10^{-4}	1.27
500 eV	0.484	0.289	0.141	0.0579	0.028	1.87

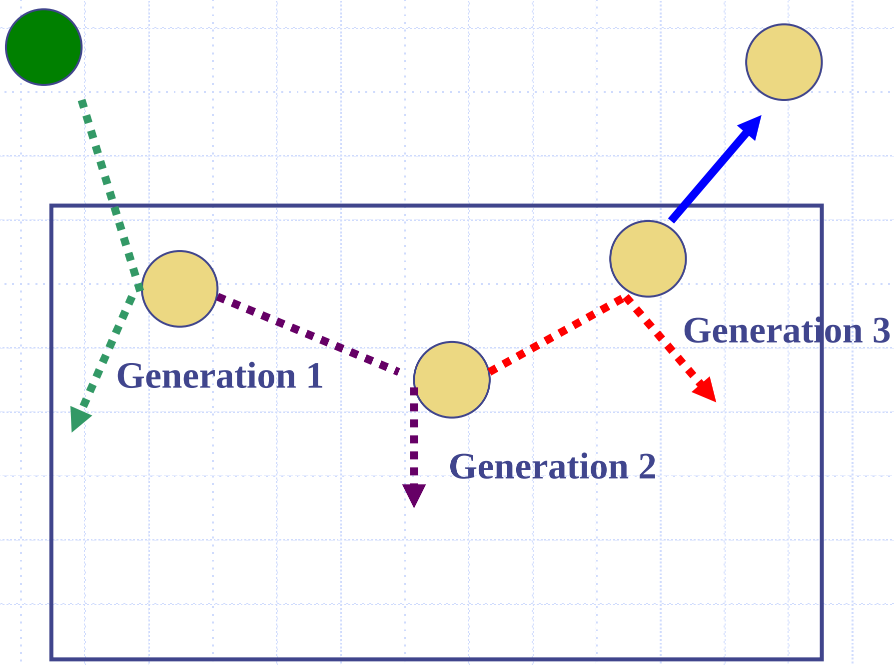
ii) $Ar^+ \rightarrow Fe$

Energy \ Generation	1	2	3	4	More than 5	Average
50 eV	0.339	0.297	0.206	0.107	0.0505	2.25
100 eV	0.280	0.306	0.230	0.117	0.0680	2.42
500 eV	0.140	0.254	0.255	0.179	0.172	3.11

Generation







Generation 1 **Generation 3**

Integral equation of primary recoil density

- **A primary recoil density $F_p(E, E_0)$ is the average number of primary recoil atoms with energy (E_0, dE_0) initiated by a light ion with energy E.**

- **Integral equation for $F_p(E, E_0)$ is the following:**

$$\int d\sigma(E,T)\left[F_P(E,E_0)-F_P(E-T,E_0)\right]+s_e(E)\frac{\partial}{\partial E}F_P(E,E_0)=\frac{\partial\sigma(E,E_0)}{\partial E_0}$$

(1)

T : energy of recoil atom, dσ : differential scattering cross-section

$s_e(E)$: electronic stopping cross-section

Solution of the integral equation

- Assumption

1) neglect the electronic energy-loss: $s_e(E)$

2) The energy transfer factor γ of the collision between a light ion and a heavy atom is small : $\gamma=4M_1M_2/(M_1+M_2)^2$

$$F_P(E-T,E_0)\approx F_P(E,E_0)-T\frac{\partial}{\partial E}F_P(E,E_0)$$

3) Power law approximation for the cross section

$$d\sigma(E,T)=CE^{-m}T^{-1-m}dT$$

- Solution

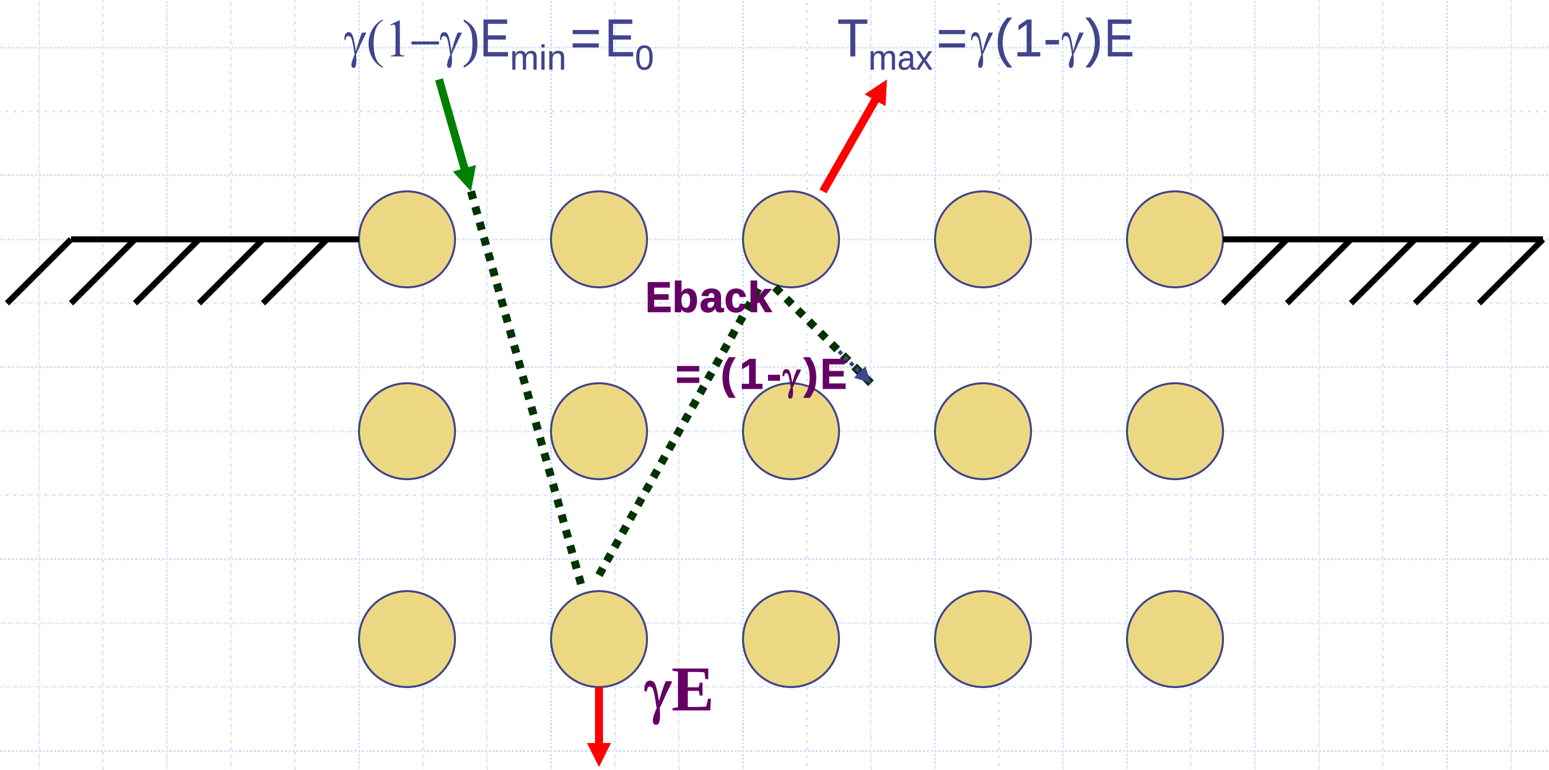
$$F_P(E,E_0) = \int_{E_{min}}^{E} dE\left[E_0^{-1-m}\Big/\int_0^{T_{max}}T^{-m}dT\right] \quad \textbf{(2)}$$

T_{max} and E_{min} of eq.(2)

T_{max}: The maximum energy of the recoil atom produced by the backscattered ion

$$T_{max}=\gamma E_{back} \qquad E_{back}=(1-\gamma)E$$

E_{min}: The minimum energy of the incident ion which produces the recoil atom with energy E_0



Solution of the integral equation

- Assumption

1) neglect the electronic energy-loss: $s_e(E)$

2) The energy transfer factor γ of the collision between a light ion and a heavy target atom is small : $\gamma=4M_1M_2/(M_1+M_2)^2$

$$F_P(E-T,E_0)\approx F_P(E,E_0)-T\frac{\partial}{\partial E}F_P(E,E_0)$$

3) Power law approximation for the cross section

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$$F_P(E,E_0) = \int_{E_{min}}^{E} dE\left[E_0^{-1-m}\Bigg/\int_0^{T_{max}} T^{-m}dT\right] \qquad \textbf{(2)}$$

Primary recoil density

- **Primary recoil density in a single knock-on cascade**

$$F_P(E,E_0)=\frac{(1-m)}{m\gamma(1-\gamma)}\left\{(T_{\max})^m E_0^{-1-m}-E_0^{-1}\right\} \qquad \textbf{(3)}$$

where

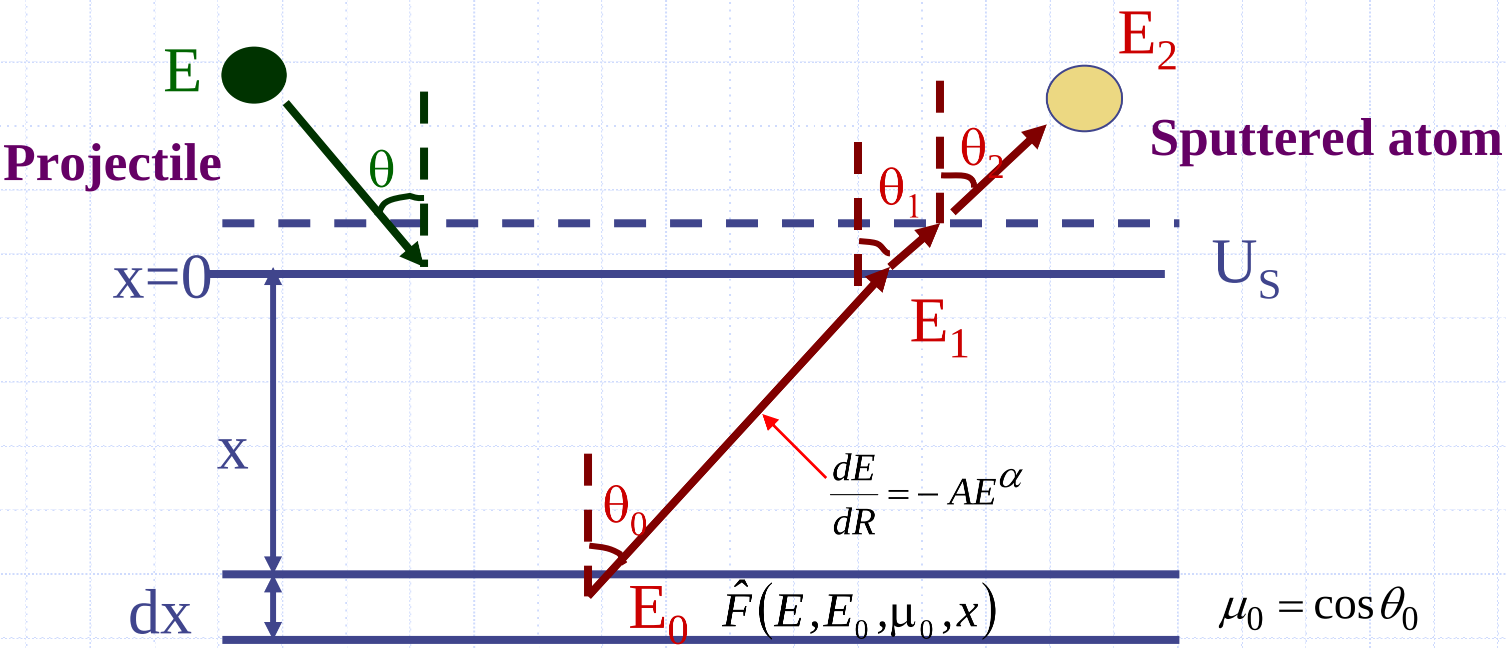
$$T_{max}=\gamma(1-\gamma)E$$

Escape & sputtering by Falcone-Sigmund model

- **Let us assume each recoil atom to slow down continuously along a straight line.**

$$\frac{dE}{dR} = -AE^{\alpha} \quad ; \quad d\sigma(E,T) = CE^{-q}T^{-1-q}dT$$

Where R : traveled path length, A : constant, α=1-2q



$J(E_1, \mu_1)dE_1d\mu_1$

The average number of the primary recoil atoms passing the surface plane with energy (E_1, dE_1) in the direction (μ_1, d μ_1) per incident ion

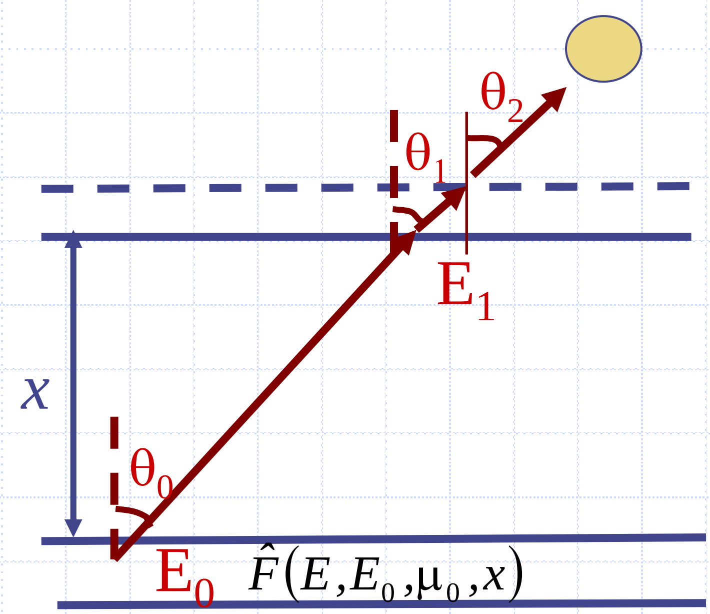
$$J(E_1,\mu_1)dE_1d\mu_1 = dE_1d\mu_1 \int_{E_1}^{T_{max}} dE_0 \int_0^{\infty} dx\hat{F}(E,\mu,E_0,x)\cdot\delta(E_1 - f(E_0,\mu_0,x)) \quad (4)$$

where

$$\mu_1 = \cos\theta_1$$

$$R_0 = \frac{E_0^{1-\alpha}}{A(1-\alpha)}$$

$$E_1 = f(E_0,\mu_0,x) = E_0\left(1-\frac{x}{R_0\cos\theta_0}\right)^{\frac{1}{1-\alpha}}$$



Assumption for primary recoil atom

- **The primary recoil atoms leading to sputtering are nearly isotopic.**

$$\hat{F}(E,E_0,\mu_0,x)dE_0 d\mu_0 dx \approx \hat{F}_p(E,E_0,x)dE_0 \frac{d\mu_0}{2} dx$$

- **Almost all of sputtered atoms are created near the surface**

$$\hat{F}_P(E,E_0,x) \approx \hat{F}_P(E,E_0,0) \approx F_P(E,E_0)$$

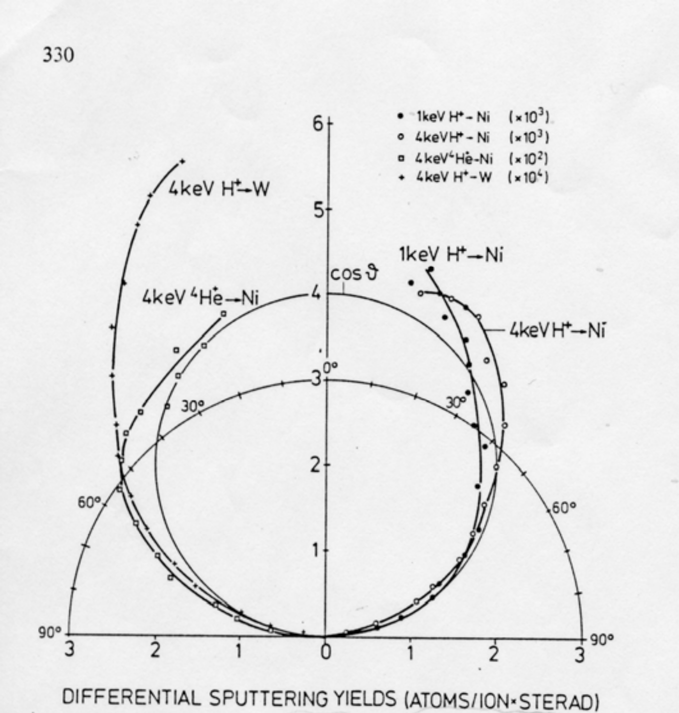


Fig. 3. Differential sputtering yields for different ion-target combinations at normal incidence. The circle is the cosine distribution

H.L.Bay, J. Bohdansky, W.O.Hofer and J. Roth, Appl. Phys. 21 (1980) 327.

- **Finally, we have**

$$J(E_1,\mu_1)dE_1 d\mu_1 = dE_1 d\mu_1 \frac{(1-m)}{2m\gamma(1-\gamma)} \frac{\cos\theta_1}{AE_1^{\alpha}} \left[\frac{1}{m} \left\{ \left(\frac{T_{\max}}{E_1} \right)^m - 1 \right\} - \ln \frac{T_{\max}}{E_1} \right] \quad \textbf{(5)}$$

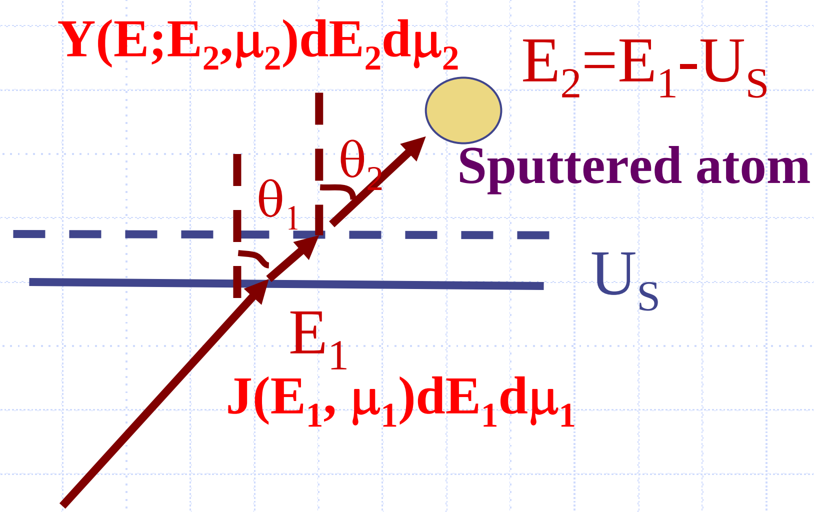
Sputtering

- An atom has to overcome a planar surface potential U_s for sputtering.

$E_1=E_2+U_s$

$E_1\cos^2\theta_1+U_s=E_2{}^2\cos\theta_2$

$\mu_2=\cos\theta_2$



$$Y(E;E_2,\mu_2)dE_2d\mu_2=dE_2d\mu_2\frac{(1-m)}{2mA\gamma(1-\gamma)}\frac{E_2\cos\theta_2}{(E_2+U_S)^{\alpha+1}}\left[\frac{1}{m}\left\{\left(\frac{T_{\max}}{E_2+U_S}\right)^m-1\right\}-\ln\frac{T_{\max}}{(E_2+U_S)}\right] \quad \textbf{(6)}$$

Integrating the above equation over μ_2

$$Y(E,E_2)dE_2=dE_2\frac{(1-m)}{2mA\gamma(1-\gamma)}\frac{E_2}{(E_2+U_S)^{\alpha+1}}\left[\frac{1}{m}\left\{\left(\frac{T_{\max}}{E_2+U_S}\right)^m-1\right\}-\ln\frac{T_{\max}}{(E_2+U_S)}\right] \quad \textbf{(7)}$$

A new formula

- Since m is enough small, then we have

$$Y(E, E_2)dE_2 \propto dE_2 \frac{E_2}{(E_2+U_S)^{\alpha+1}} \left[\ln \frac{T_{max}}{E_2+U_S} \right]^2 \qquad \textbf{(8)}$$

- α=3/5 corresponds to q=1/5

(literature values on q* : 0.1 – 0.34)

$$Y(E, E_2)dE_2 \propto dE_2 \frac{E_2}{(E_2+U_S)^{8/5}} \left[\ln \frac{T_{max}}{E_2+U_S} \right]^2 \qquad \textbf{(9)}$$

where $T_{max} = \gamma(1-\gamma)E$

* M. Nastasi et al.,” *Ion-Solid Interactions: Fundamentals and applications*” (Cambridge University Press 1996, in Cambridge), p83.

Three formulae for the energy spectrum of sputtered atoms

- Present formula

$$Y(E,E_2)dE_2 \propto dE_2 \frac{E_2}{(E_2+U_S)^{8/5}}\left[\ln\frac{\gamma(1-\gamma)E}{E_2+U_S}\right]^2$$

- Thompson formula

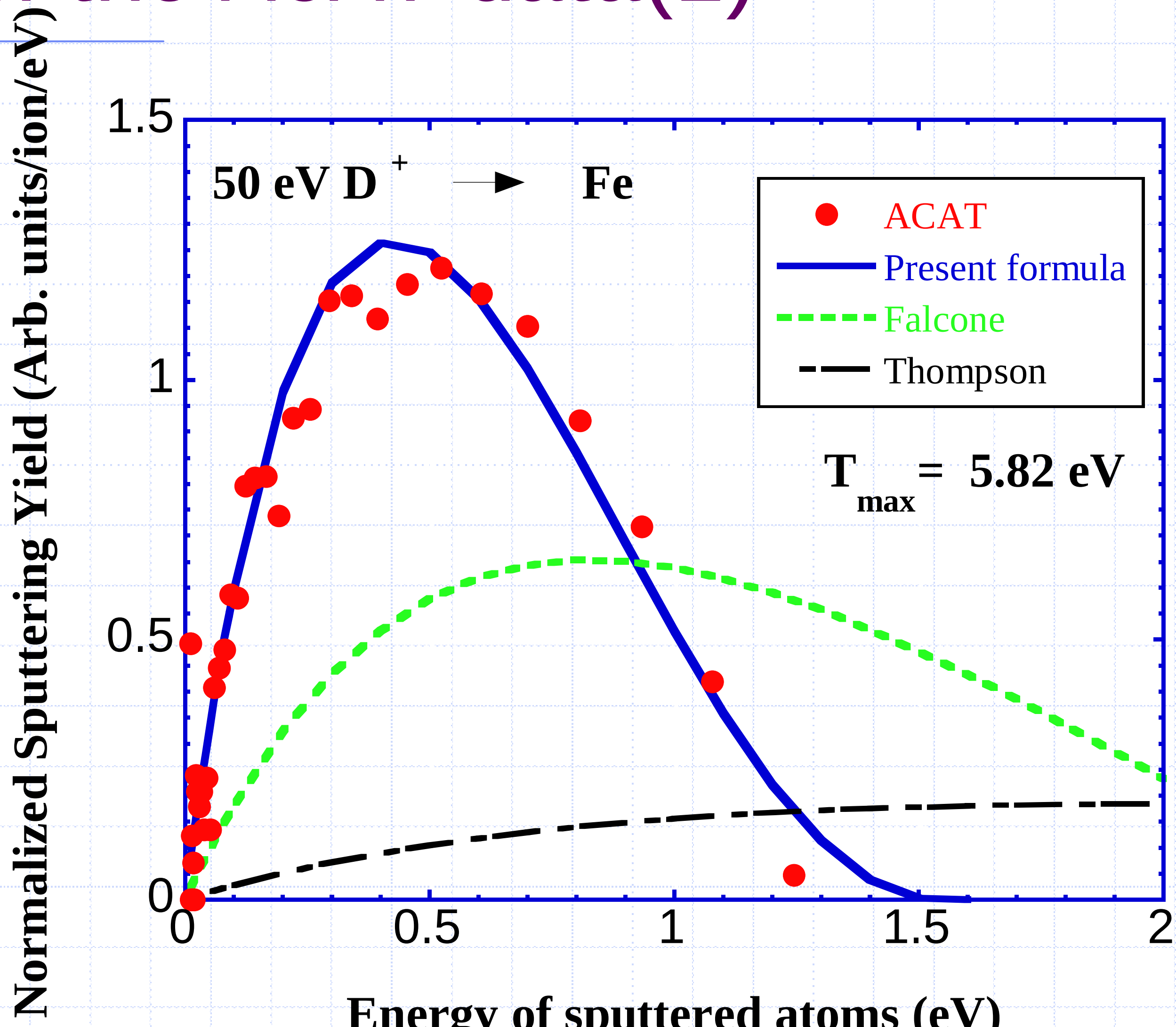
$$Y(E_2)dE_2 \propto \frac{E_2}{(E_2+U_S)^3}dE_2$$

- Falcone formula

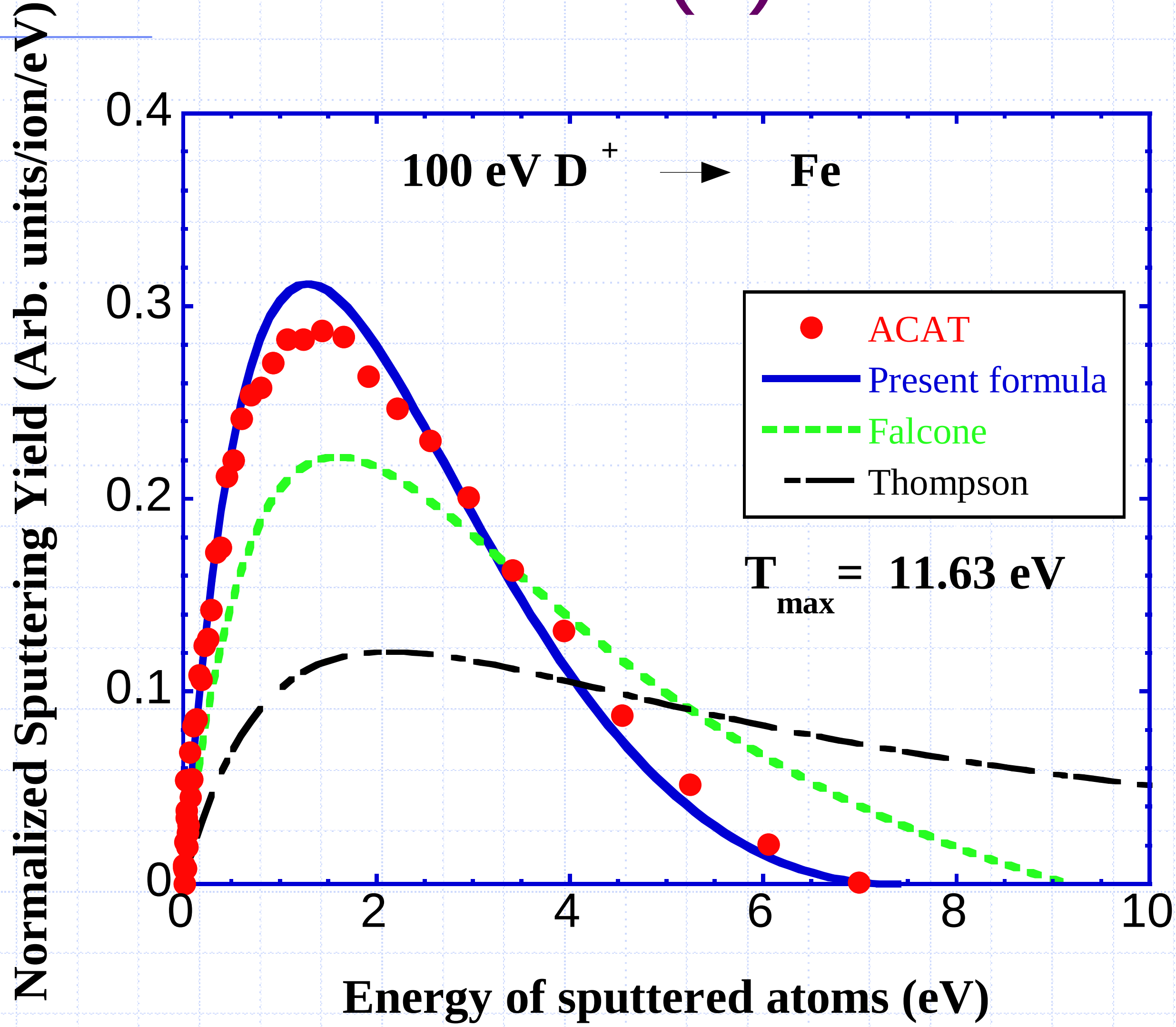
$$Y(E,E_2)dE_2 \propto dE_2 \frac{E_2}{(E_2+U_S)^{5/2}}\ln\frac{\gamma E}{E_2+U_S}$$

* G. Falcone, Surf. Sci. 187 (1987) 212

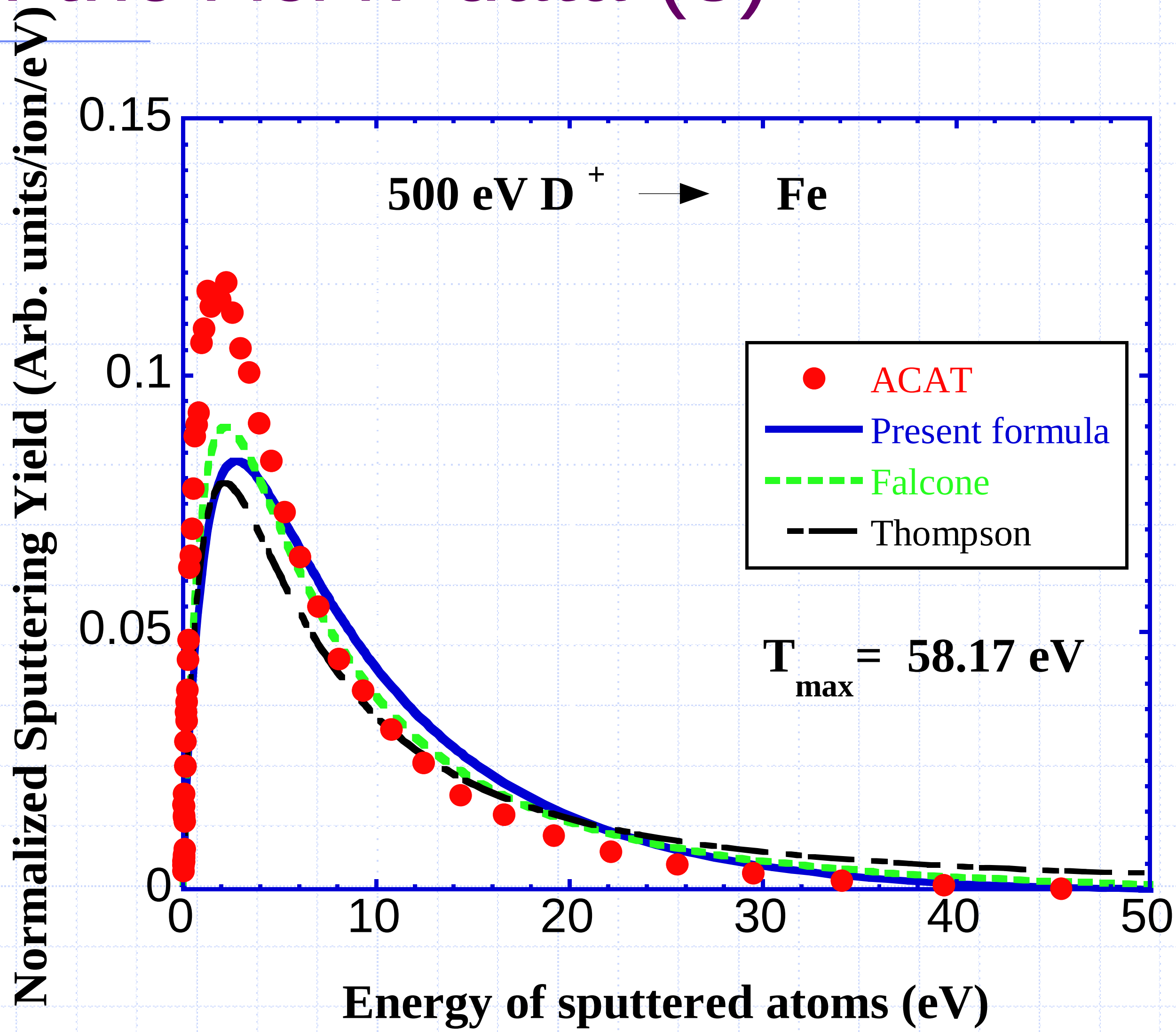
Comparison of the present formula with the ACAT data(1)



Comparison of the present formula with the ACAT data (2)



Comparison of the present formula with the ACAT data (3)



Summery

- The peak energy of the energy spectrum of $D^+ \rightarrow Fe$

E	ACAT	Present work	Falcone	Thompson
50 eV	0.5eV	0.43eV	0.83eV	2.14eV
100 eV	1.3eV	1.29eV	1.58eV	2.14eV
500 eV	1.8eV	2.77eV	2.22eV	2.14eV

- 50 eV and 100 eV are good.
- 500 eV is not good
  1) The electronic energy loss should be included.
  2) The recoils with the higher-order generation are sputtered.

ACAT code

- Monte Calro Method
- Binary Collision approximation
- Amorphous Target
- Unite Cell

（$R_0 = N^{-1/3}$、N：a number density of a target material）