Calculations and Measurements of Electron Inelastic Mean Free Paths in Solids

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1. Introduction

- The electron inelastic mean free path (IMFP) is a basic material parameter for describing the surface sensitivity of AES, XPS and other surface electron spectroscopies.
- growing interest in XPS and related experiments performed with X-rays of much higher energies for both scientific and industrial purposes. (up to 30keV)
- a need for IMFPs at higher energy region in transmission electron microscopy. (up to 200 or 300 KeV)

We started to extend the IMFP calculations over 10 eV to 200 keV using relativistic full Penn algorithm (FPA) from ELFs for 41 elemental solids and 30 compound semiconductors.

2. Calculation of IMFPs from optical data
- IMFP calculation with relativistic full Penn algorithm

:Relativistic DCS (< 0.5 MeV; Fernandez-Varea)

$$\frac{d^2\sigma}{d\omega dq} = \frac{d^2\sigma_L}{d\omega dq} + \frac{d^2\sigma_T}{d\omega dq} \approx \frac{d^2\sigma_L}{d\omega dq} = \frac{2}{\pi N v^2} \mathrm{Im}\left(\frac{-1}{\varepsilon(q,\omega)}\right)\frac{1}{q}$$

: Probability *P(T,ω)* for energy loss per unit distance traveled by an electron with relativistic kinetic energy *T*.

$$p(T,\omega) = \frac{\left(1+T/c^2\right)^2}{1+T/\left(2c^2\right)} \frac{1}{\pi T} \int_{q_-}^{q_+} \frac{dq}{q} \mathrm{Im}\left[\frac{-1}{\varepsilon(q,\omega)}\right]$$

$$q_\pm = \sqrt{T\left(2+T/c^2\right)} \pm \sqrt{(T-\omega)\left(2+(T-\omega)/c^2\right)}$$

$$\lambda(T) = 1 / \int_0^{\omega_{\max}} p(T,\omega)\ d\omega$$

Full Penn Algorithm for ELF calculation

The ELF in the FPA can be expressed as:

$$\mathrm{Im}\left[\frac{-1}{\varepsilon(q,\omega)}\right] = \int_0^\infty d\omega_p g(\omega_p)\,\mathrm{Im}\left[\frac{-1}{\varepsilon^L(q,\omega;\omega_p)}\right]$$

← Lindhard ELF

$$g(\omega) = \frac{2}{\pi\omega}\mathrm{Im}\left[\frac{-1}{\varepsilon(\omega)}\right]$$

← Optical ELF (measured)

$$\mathrm{Im}\left[\frac{-1}{\varepsilon^L(q,\omega;\omega_p)}\right] = \frac{\varepsilon_2^L}{(\varepsilon_1^L)^2 + (\varepsilon_2^L)^2}$$

$$\varepsilon_1^L(q,\omega;\omega_p) = 1 + \frac{1}{\pi k_F z^2}\left[\frac{1}{2} + \frac{1}{8z}\left\{F\left(z - \frac{x}{4z}\right) + F\left(z + \frac{x}{4z}\right)\right\}\right]$$

$$\varepsilon_2^L(q,\omega;\omega_p) = \frac{1}{8k_F z^3} \times \begin{cases} x & \text{for } 0 < x < 4z(1-z) \\ 1-(z-(x/4z))^2 & \text{for } |4z(1-z)| < x < 4z(1+z), \\ 0 & \text{otherwise} \end{cases}$$

Conditions and materials for IMFP calculations

Energy range for IMFP calculations: 10 eV to 200 keV
- calculated at equal intervals on a logarithmic energy scale corresponding to increases of 10 %.

Energy range of ELFs for materials: 0.1 eV - 1MeV

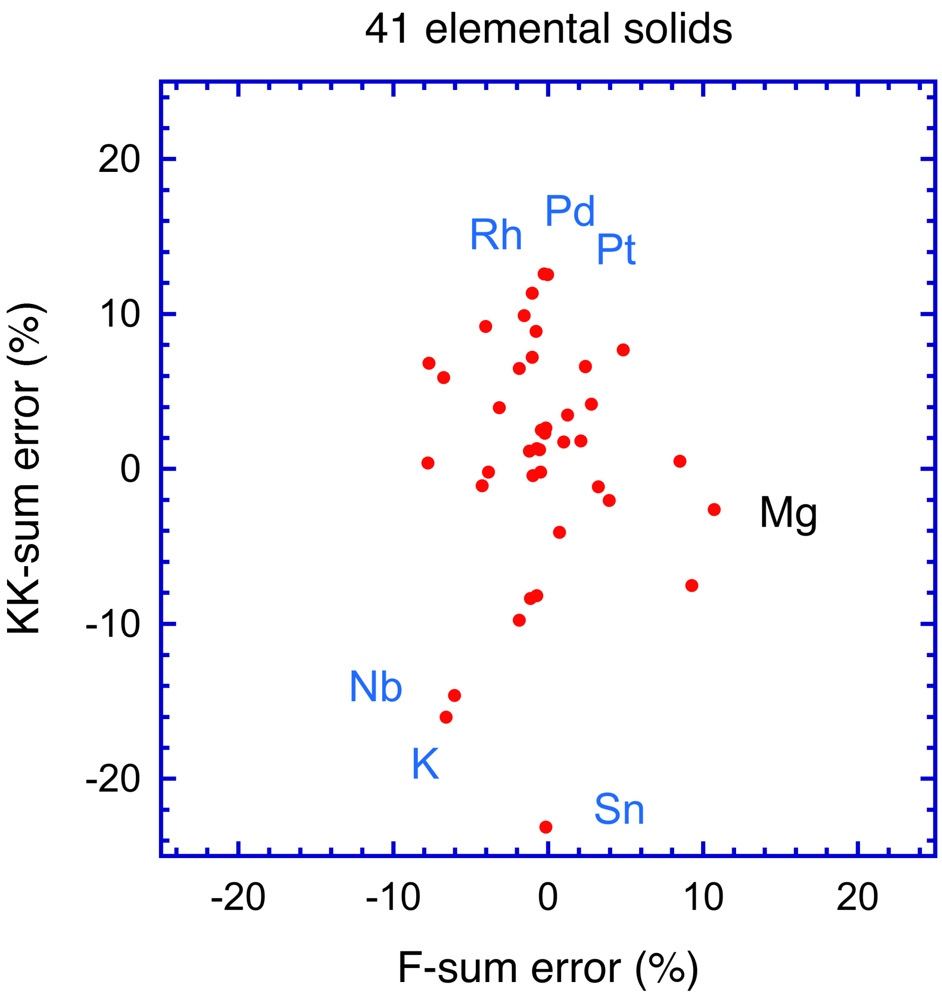
- 41 elemental solids

Li, Be, diamond, graphite, glassy carbon, Na, Mg, Al, Si, K, Sc, Ti, V, Cr, Fe, Co, Ni, Cu, Ge, Y, Nb, Mo, Ru, Rh, Pd, Ag, In, Sn, Cs, Gd, Tb, Dy, Hf, Ta, W, Re, Os, Ir, Pt, Au, and Bi.

-30 compound semiconductors

AgBr, AgCl, AgI, AlAs, AlN, AlSb, BN, BN(hex), CdS, CdSe, CdSe(hex), CdTe, GaAs, GaN, GaP, GaSb, GaSe, InAs, InP, InSb, PbS, PbSe, PbTe, SiC, SiC(hex), SnTe, ZnS, ZnS(hex), ZnSe, ZnTe

Evaluation of ELFs (0 - 1MeV) : elemental solids



- F-sum : One solid is slightly larger than 10 % (Mg) .
- KK-sum : 6 solids are larger than 10 % error (K, Nb, Rh, Pd, Sn, and Pt).

- the sum-rule errors for K and Nb are both of the same sign (negative in each case), indicating that <u>their ELFs are systematically too small and thus their calculated IMFPs will be too large.</u>

- For 34 of our 41 elemental solids, the f-sum-rule and KK-sum rule errors are both less than 10 %.

ELFs : compound semiconductor

·Experimental ELFs or optical constants are lacking over 10 eV.

- Optical Constants and ELFs for 30 compound semiconductors were calculated with **FEFF8.2 and WIEN2K in 0.1 eV – 1 MeV**.

FEFF: Automated program to calculate the X-ray absorption spectra based on an ab initio all-electron, real space relativistic Green's function formalism
→ Available for inner-shell electron excitation

WIEN2K: Program package to perform the electron structure calculation based on density functional theory using full potential and linearized augmented plane wave method
→Available for valence electron excitation

- Space group and cell parameters : ex. AgBr , F m -3 m, a = 5.775

List of 30 semiconductors calculated

Material	Space Group	Cell parameter (angstrom or degree)
AgBr	F m -3 m	a = 5.775
AgCl	F m -3 m	a = 5.543
AgI	P 63 m c	a = 4.5856 c = 7.49 g = 120
AlAs	F -4 3 m	a = 5.6605
AlN	P 63 m c	a = 3.11 c = 4.98 g = 120
AlSb	F -4 3 m	a = 6.135
BN	F -4 3 m	a = 3.6159
BN_hex	P 63 /mmc	a = 2.5045 c = 6.606 g = 120
CdS	P 63 m c	a = 4.142 c = 6.724 g = 120
CdSe	F -4 3 m	a = 6.04
CdSe_hex	P 63 m c	a = 4.299 c = 7.01 g = 120
CdTe	F -4 3 m	a = 6.482
GaAs	F -4 3 m	a = 5.6532

Material	Space Group	Cell parameter (angstrom or degree)
GaN	P 63 m c	a = 3.1891 c = 5.1855 g = 120
GaP	F -4 3 m	a = 5.4508
GaSb	F -4 3 m	a = 6.0959
GaSe	P 63 /mmc	a = 3.75 c = 15.995 g = 120
InAs	F -4 3 m	a = 6.0577
InP	F -4 3 m	a = 5.8687
InSb	F -4 3 m	a = 6.4794
PbS	F m -3 m	a = 5.9315
PbSe	F m -3 m	a = 6.1213
PbTe	F m -3 m	a = 6.4541
SiC	F -4 3 m	a = 4.3581
SiC_hex	P 63 m c	a = 3.076 c = 5.048 g = 120
SnTe	F m -3 m	a = 6.323
ZnS	F -4 3 m	a = 5.4102
ZnS_hex	P 63 m c	a = 3.822 c = 6.26 g = 120
ZnSe	F -4 3 m	a = 5.6692
ZnTe	F -4 3 m	a = 6.1026

Optical constants by FEFF

✓Input: Crystal structure

✓Phot absorption cross section from all absorption edge by the use of XANES, EXAFS, FPRIME card→ Total absorption spectrum μ(ω)

✓X-ray scattering factor f_2 and f_1 (by Kramers-Kronig relation)

$$f_1(\omega) = Z + \frac{1}{2\pi^2 r_0 c} \mathrm{P.}\int_0^\infty d\omega' \frac{\omega'^2 \mu(\omega')}{\omega^2 - \omega'^2}$$

$$f_2(\omega) = \frac{\omega}{4\pi r_0 c} \mu(\omega)$$

✓Optical constants n and k

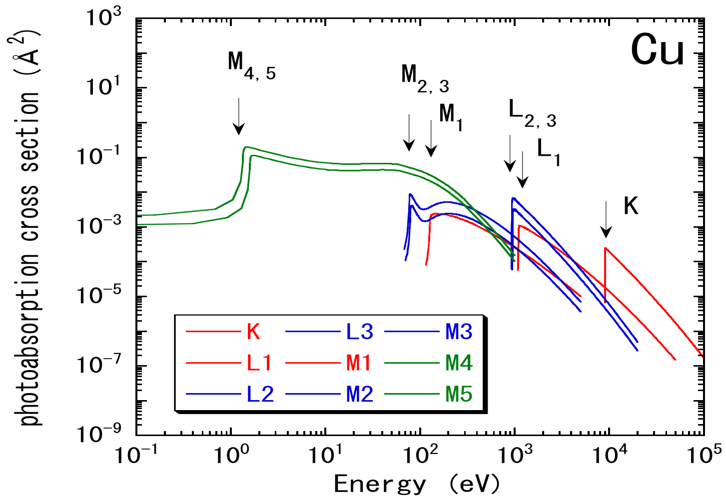
$$n = 1 - \frac{r_0 \lambda^2}{2\pi} \rho f_1, \qquad k = \frac{r_0 \lambda^2}{2\pi} \rho f_2$$

Dielectric function and Energy loss function

$$\varepsilon = \varepsilon_1 + i\varepsilon_2$$
$$\varepsilon_1 = n^2 - k^2, \quad \varepsilon_2 = 2nk$$

$$-\mathrm{Im}[1/\varepsilon] = \frac{\varepsilon_2}{\varepsilon_1^2 + \varepsilon_2^2}$$

Ex. Photoabsorption cross section of Cu



Z: atomic number
ω: angular frequency
r_0: classical electron radius
c: velocity of light
ρ: density of solid

Optical Constants by WIEN2k

✓Input: Crystal structure

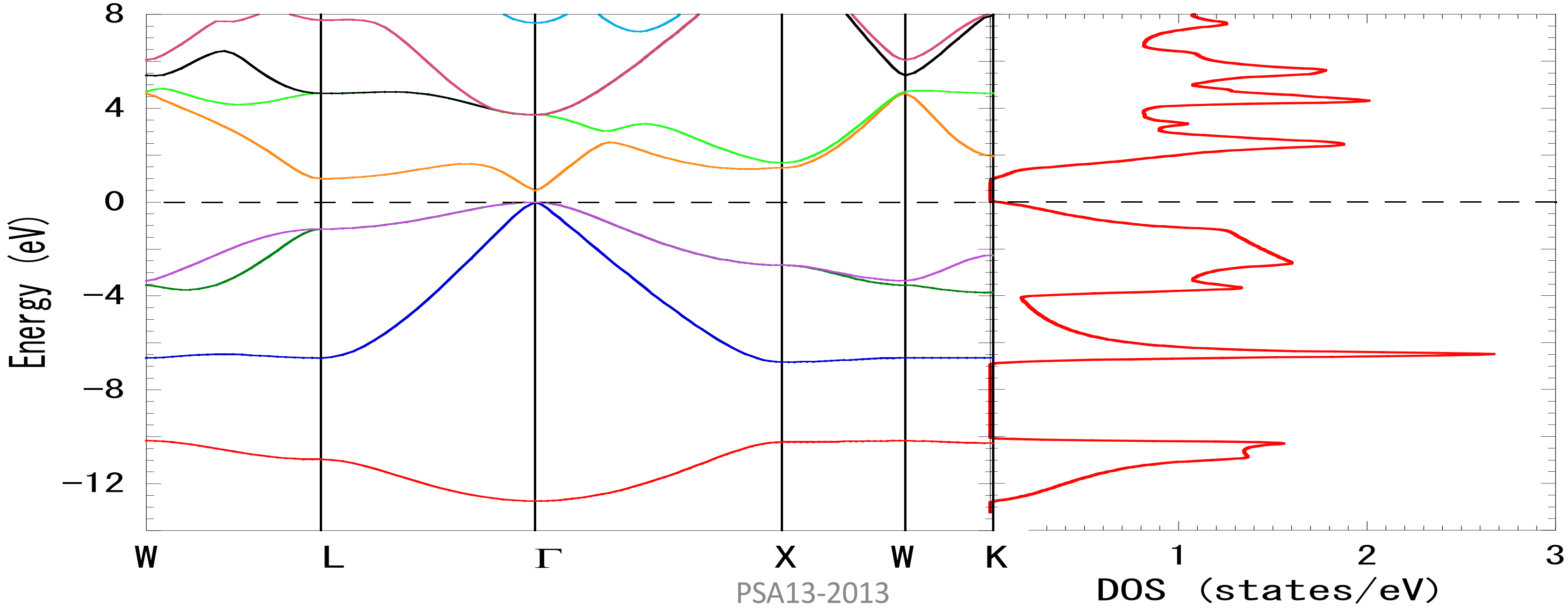
↓

✓SCF calculation

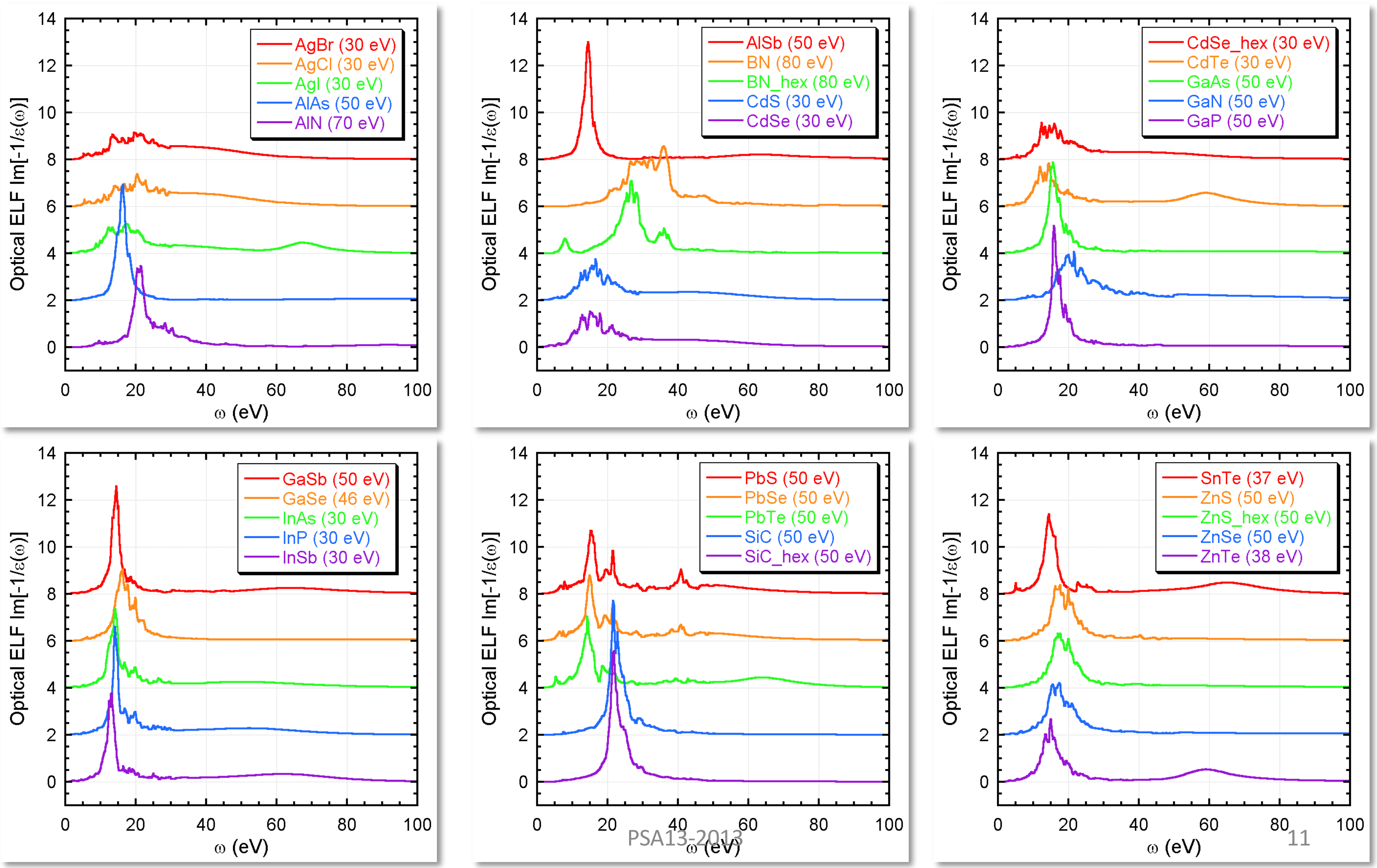
↓

✓Dielectric function and Optical constants

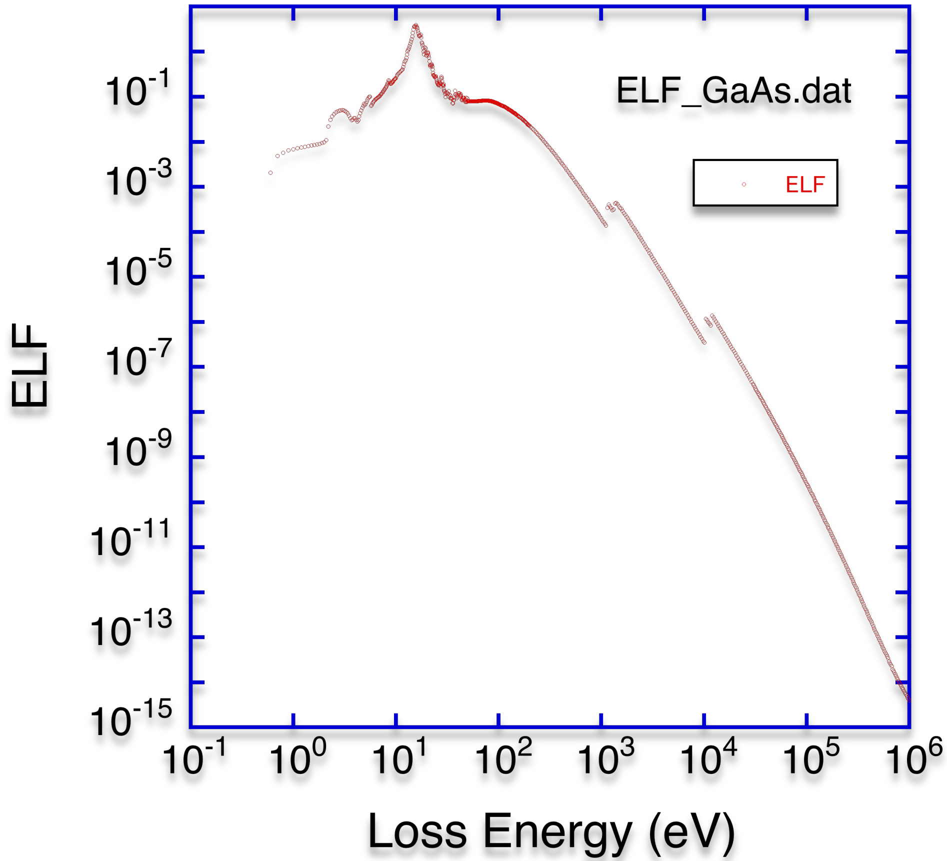
ex. Band structure and DOS of GaAs



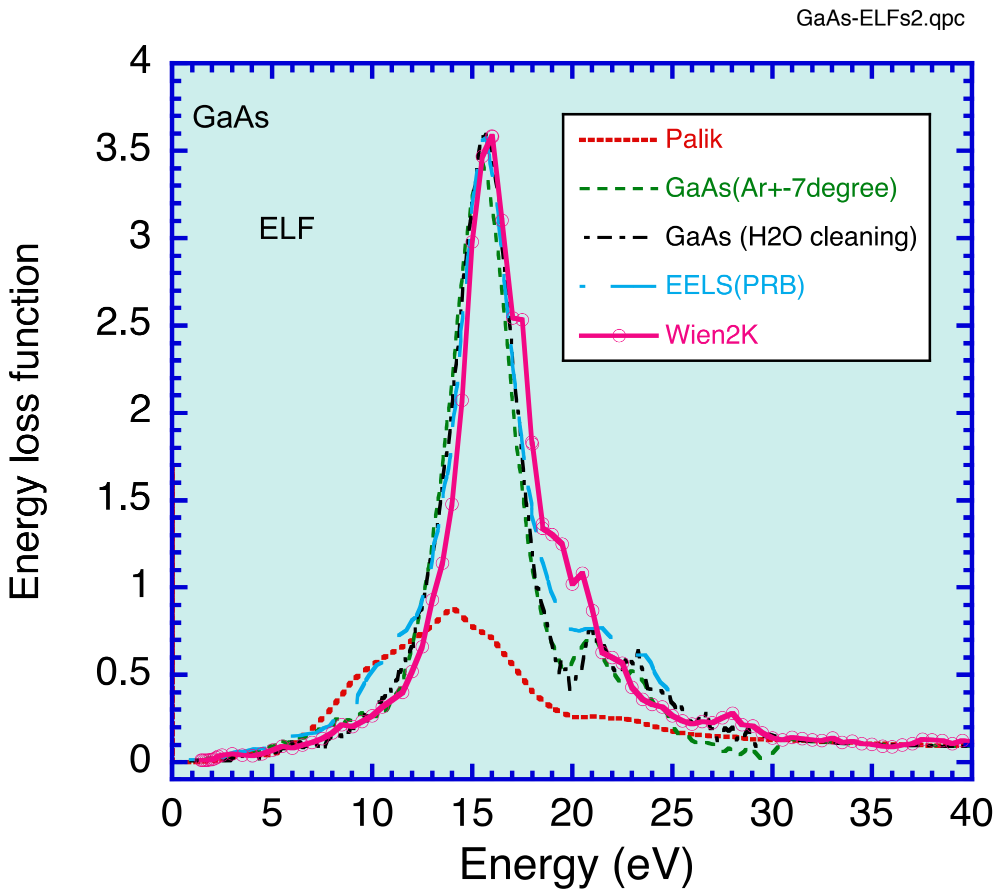
Calculated results of ELFs for 30 compounds: 0 -100 eV



ELF for GaAs

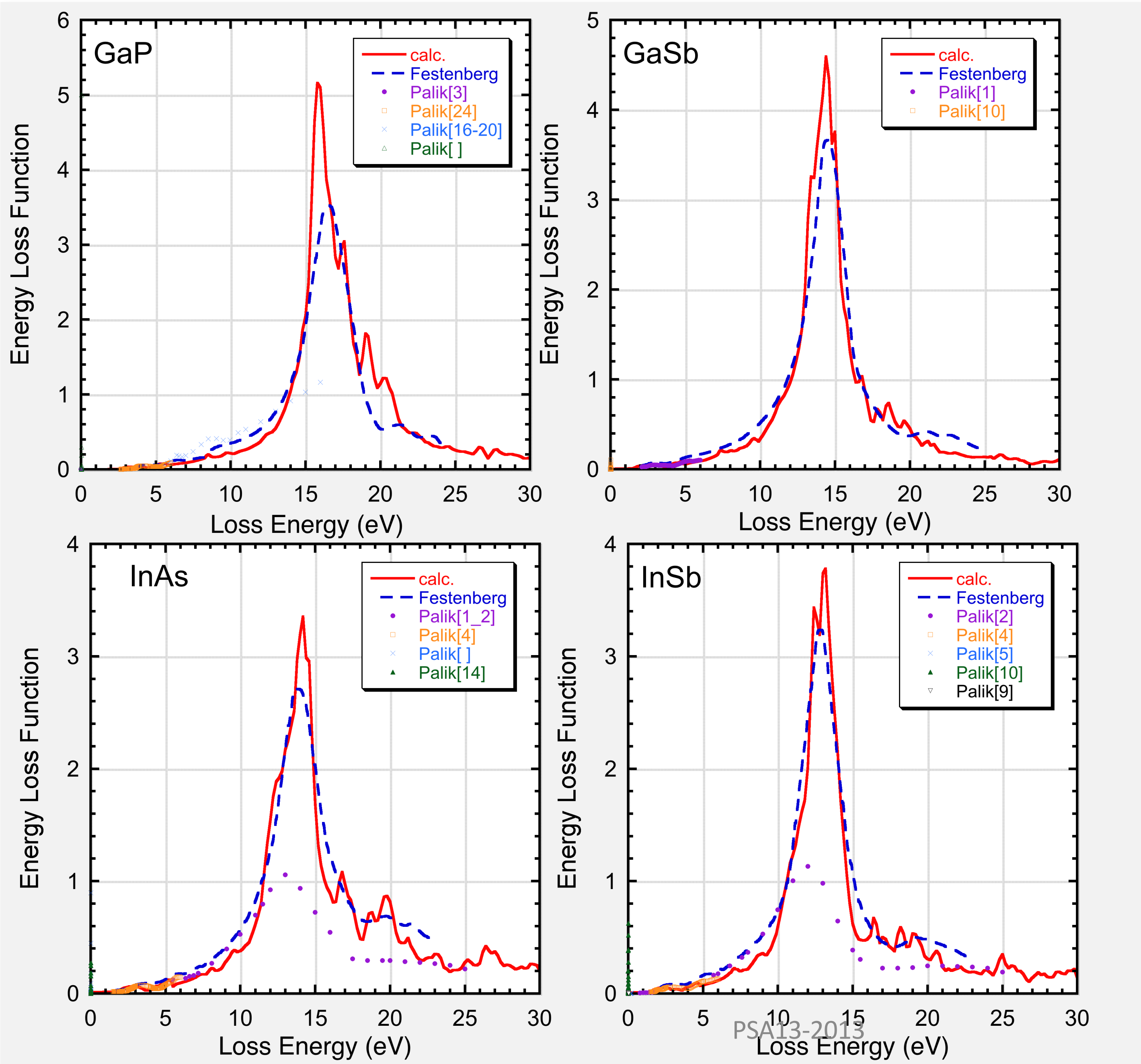


Resulting ELF of GaAs : Wien2K + FEEE



Comparison of ELFs from REELS

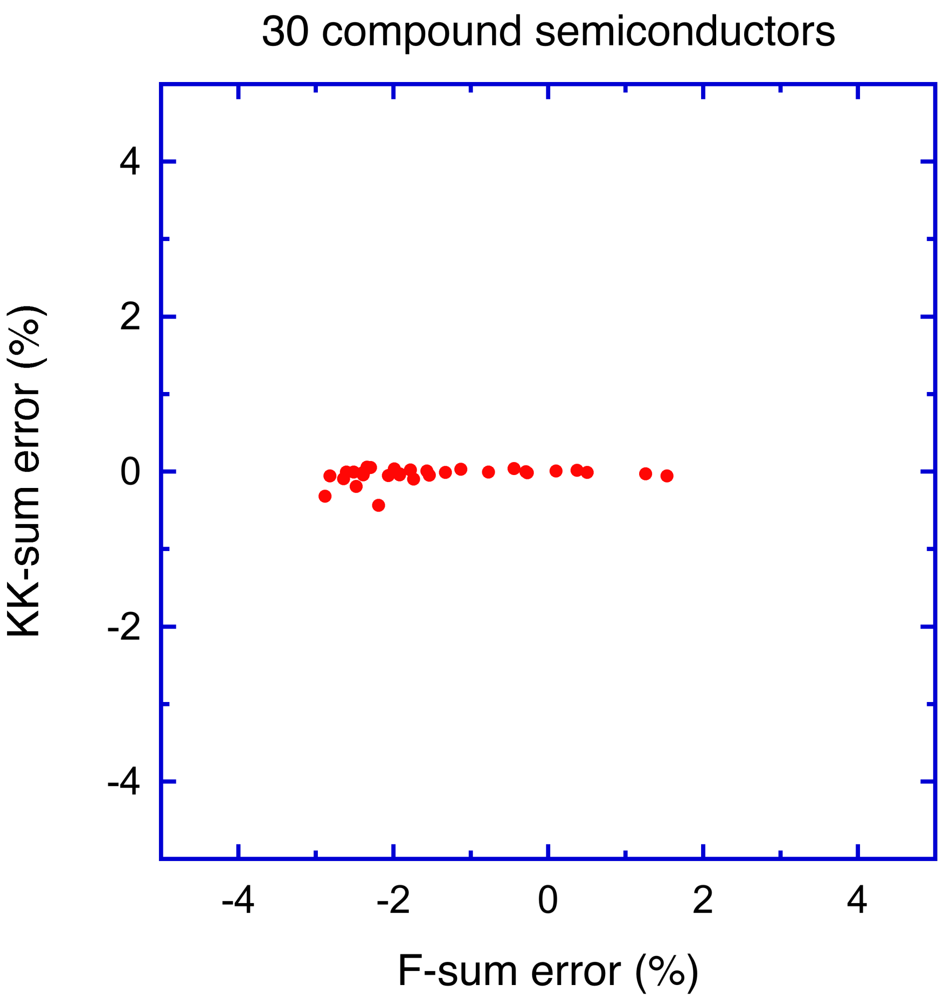
Comparison of ELFs with Palik and Festenberg data

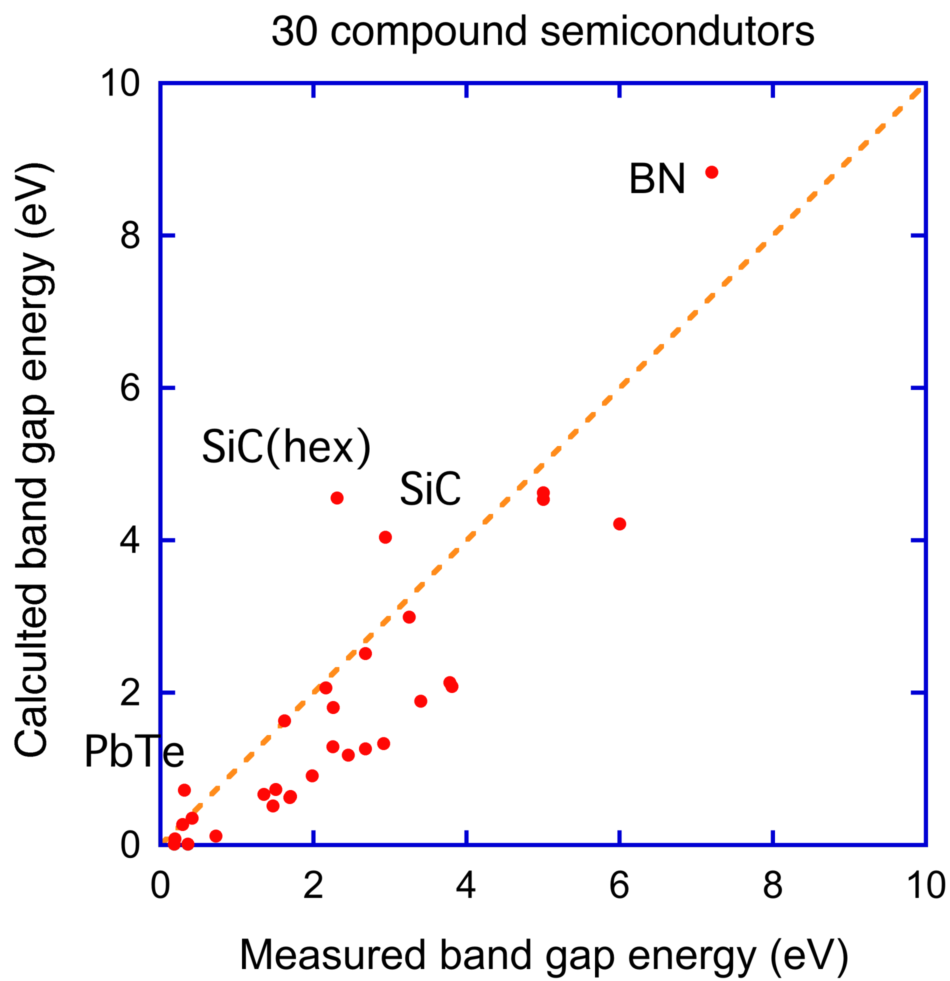


: good agreement
Wien2k - TEM

: poor >10 eV (InAs,InSb)
Wien2k – Palik data

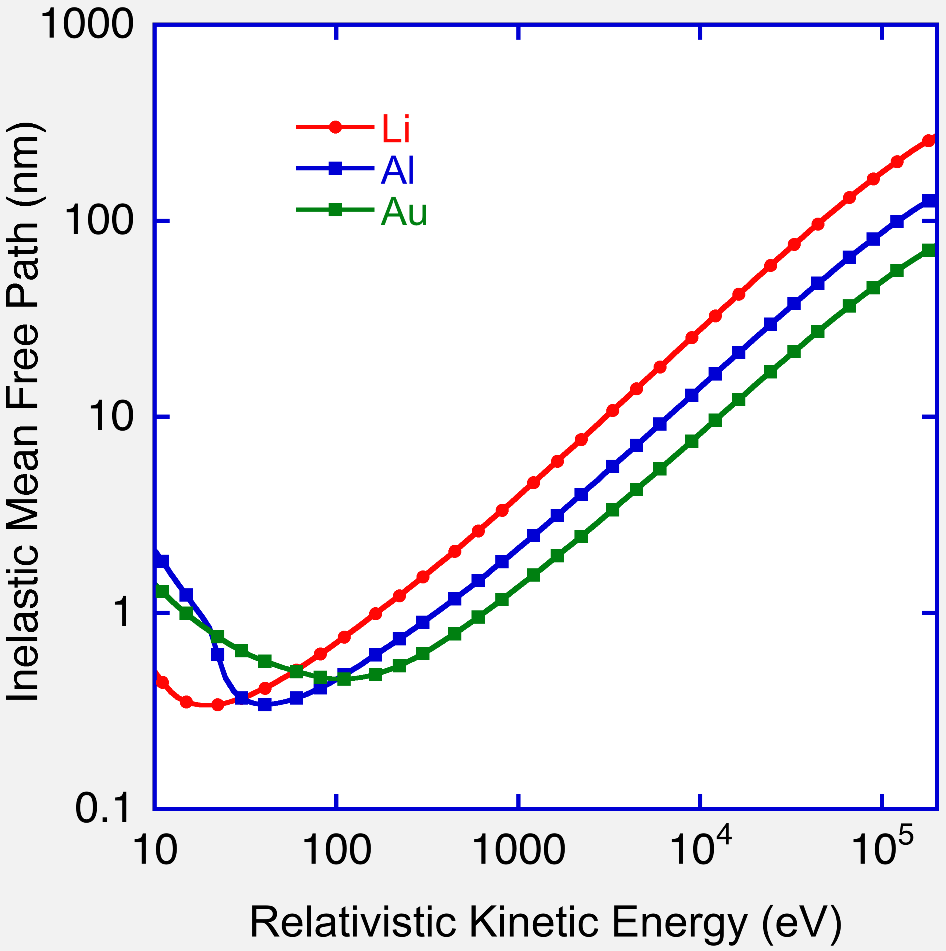
Evaluation of ELFs : 30 compound semiconductors

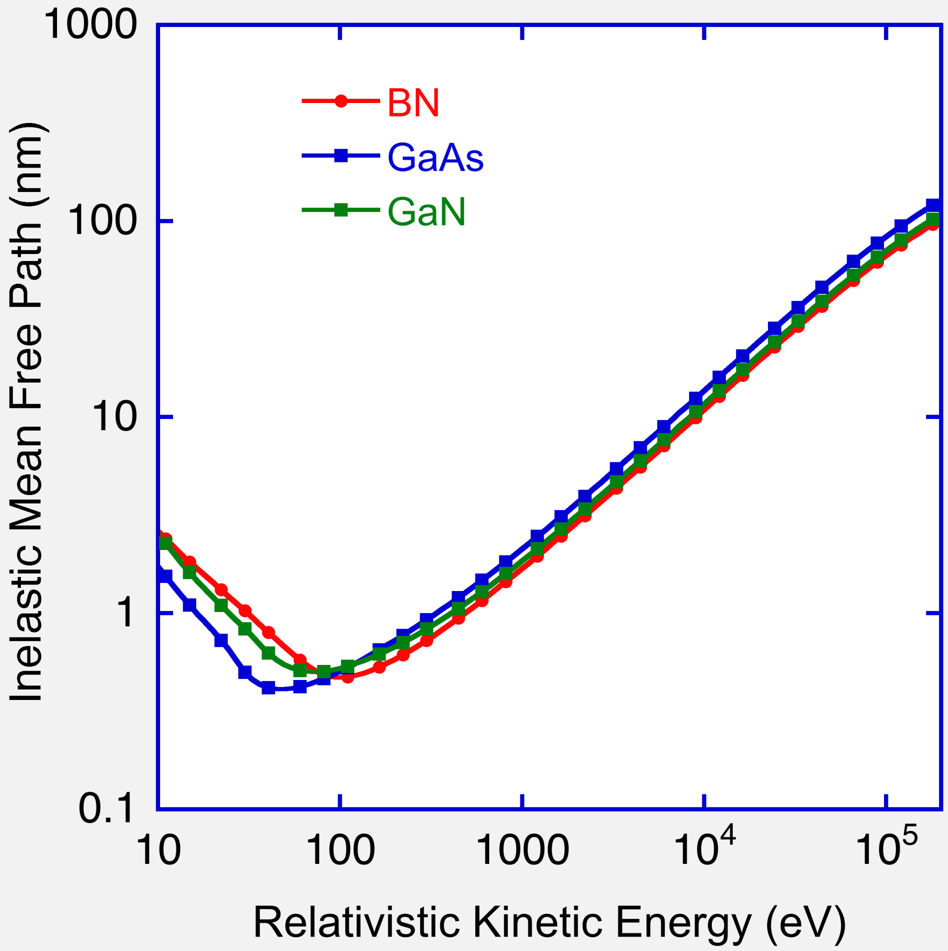




Calculated Eg : estimated from calculated ELFs
Measured Eg : median value in the references

Calculated results of IMFPs : 10 eV – 200keV





Relativistic TPP-2M eq. and Fano Plot

$$\sigma_{tot} = \frac{4\pi a_0^2 z^2}{mv^2/2R}\left\{M_{tot}^2\left[\ln\left(\frac{4c_{tot}}{R}\frac{mv^2}{2}\right) - \ln\left(1-B^2\right) - B^2\right]\right\}$$

Relativistic Bethe equation by Inokuti

$$B = \frac{v}{c}$$

Non-relativistic Bethe equation

$$\sigma_{tot}^{non-rel} = \frac{4\pi a_0^2 z^2}{E/R}\left\{M_{tot}^2\left[\ln\left(\frac{4c_{tot}E}{R}\right)\right] + \frac{g_n}{E/R} + O\left(\frac{h_n}{E^2}\right)\right\}$$

$$\lambda^{non-rel} = \frac{E}{E_p^2\left\{\beta\ln(\gamma E) - C/E + D/E^2\right\}} \quad \text{(nm)}$$

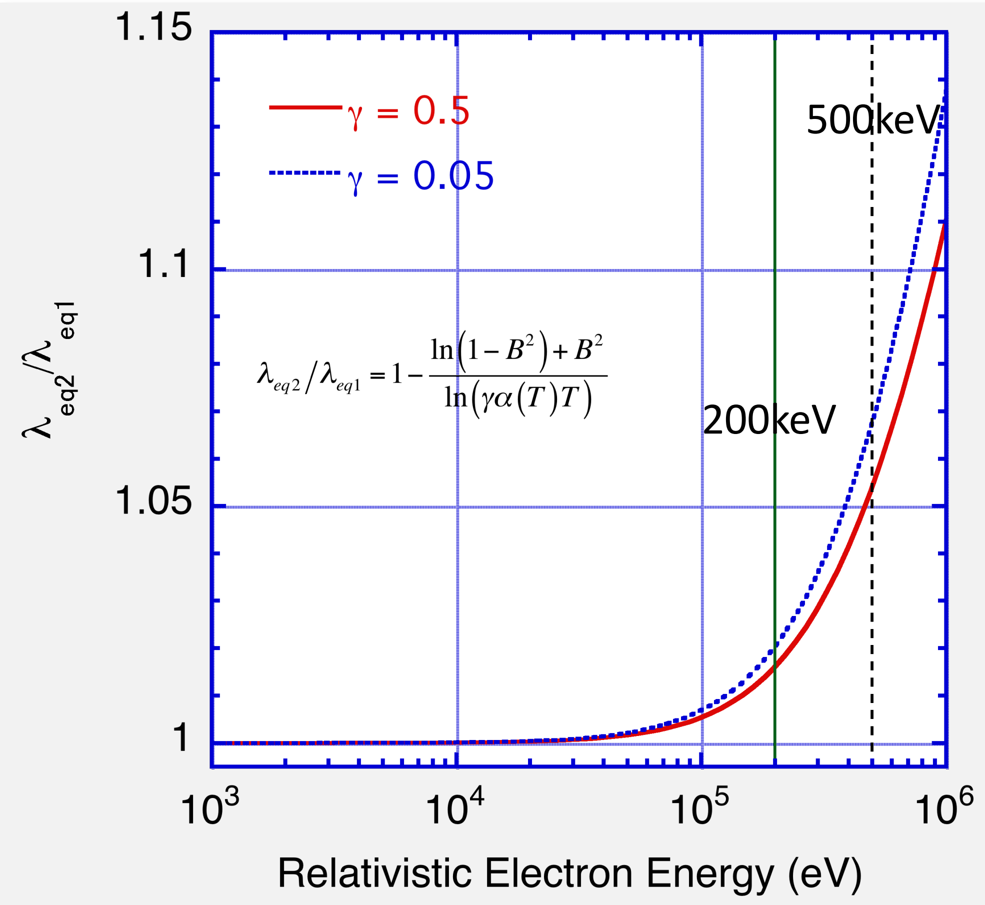
$$\lambda = \frac{\alpha(T)T}{E_p^2\left\{\beta\left[\ln\left(\gamma\alpha(T)T\right) - \ln\left(1-B^2\right) - B^2\right] - C/T + D/T^2\right\}} \quad \text{(nm)}$$

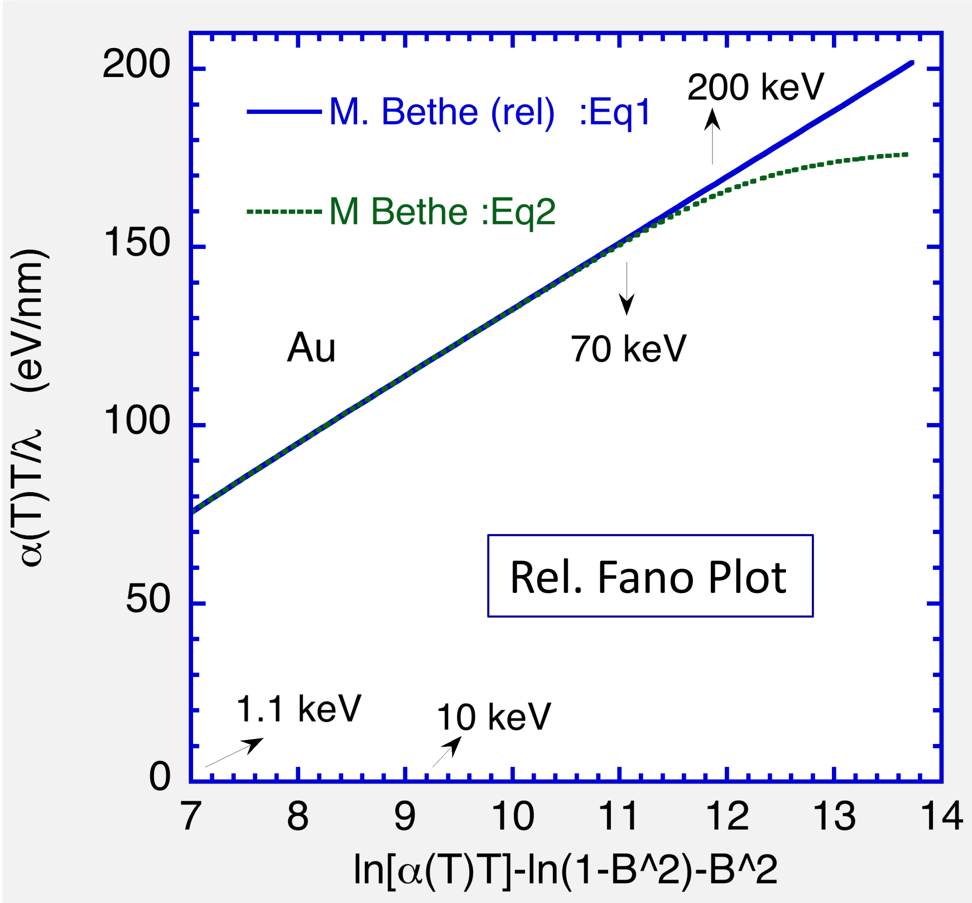
$$\alpha(T) = \frac{1 + T/\left(2m_e c^2\right)}{\left[1 + T/\left(m_e c^2\right)\right]^2}$$

Relativistic Fano plot : $\alpha(T)T/\lambda \quad vs. \quad \left[\ln\left(\alpha(T)T\right) - \ln\left(1-B^2\right) - B^2\right]$

Straight line at high energy region : γ = slope

Comparison of eq.1 and 2 on Fano plot





Eq.1

$$\lambda_{eq1} = \frac{\alpha(T)T}{E_p^{\,2}\left\{\beta\left[\ln\left(\gamma\alpha(T)T\right)-\ln\left(1-B^2\right)-B^2\right]-C/T+D/T^2\right\}}$$

Eq.2

Original M. Bethe eq. form

$$\lambda_{eq2} = \frac{\alpha(T)T}{E_p^{\,2}\left\{\beta\ln\left(\gamma\alpha(T)T\right)-C/T+D/T^2\right\}}$$

Fano plots of Au over 1keV – 1MeV

:Relativistic DCS

longitudinal excitation

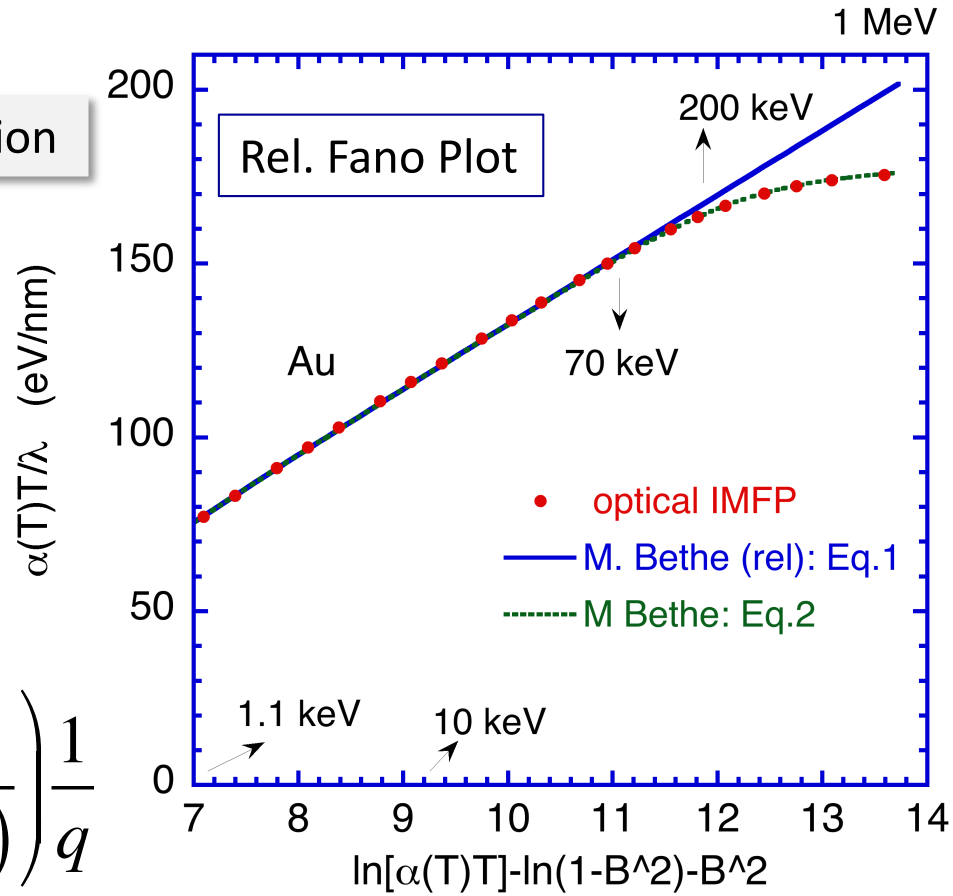
transverse excitation

$$\frac{d^2\sigma}{d\omega dq} = \frac{d^2\sigma_L}{d\omega dq} + \frac{d^2\sigma_T}{d\omega dq}$$

$$\lambda^{-1} = n\sigma$$

< 0.5 MeV

$$\frac{d^2\sigma}{d\omega dq} \simeq \frac{d^2\sigma_L}{d\omega dq} = \frac{2}{\pi N v^2}\,\mathrm{Im}\left(\frac{-1}{\varepsilon(q,\omega)}\right)\frac{1}{q}$$



Eq.1

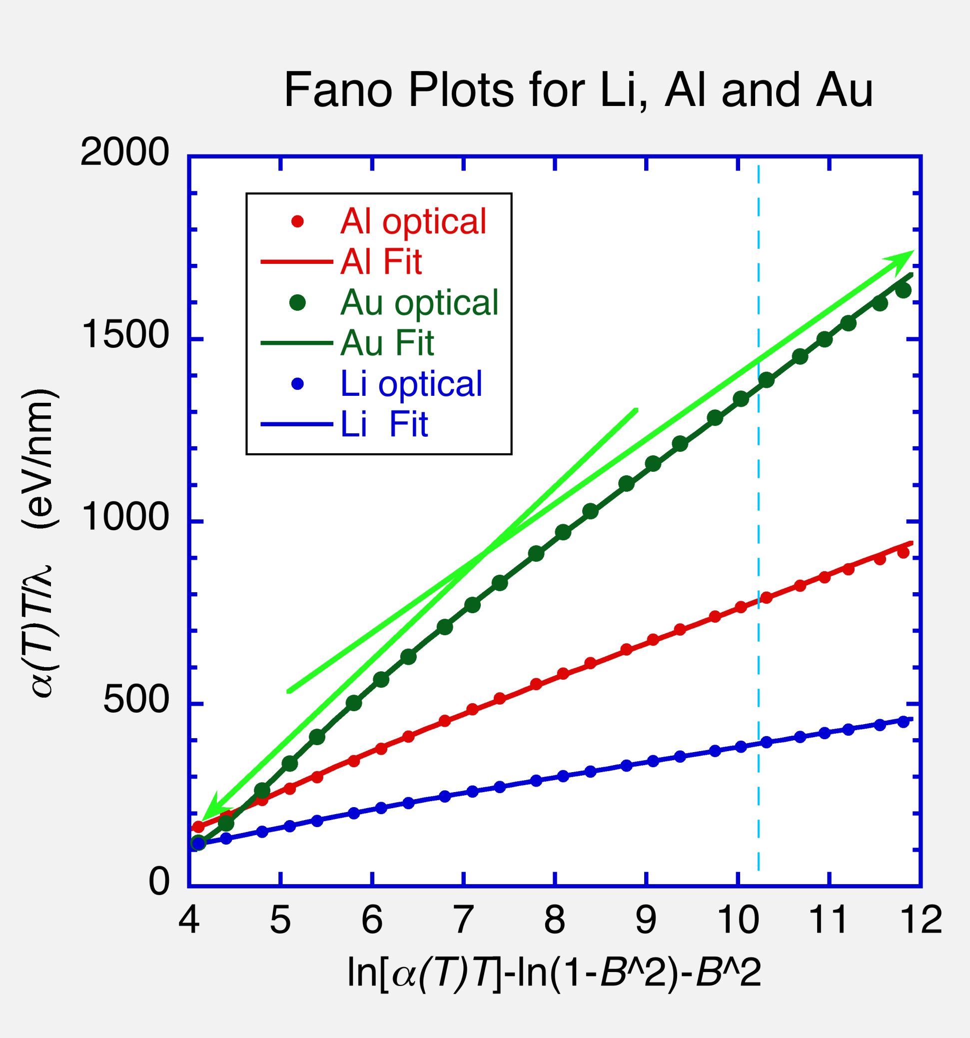
$$\lambda_{eq1} = \frac{\alpha(T)T}{E_p^{\,2}\left\{\beta\left[\ln\left(\gamma\alpha(T)T\right) - \ln\left(1-B^2\right) - B^2\right] - C/T + D/T^2\right\}}$$

Eq.2

Original M. Bethe eq. form

$$\lambda_{eq2} = \frac{\alpha(T)T}{E_p^{\,2}\left\{\beta\ln\left(\gamma\alpha(T)T\right) - C/T + D/T^2\right\}}$$

Fano plots and Curve fits for 3 elemental solids



Solid circles: calculated from IMFPs (rel. FPA method)

Solid lines: Fit with Rel. mod. Bethe equation

Energy range: 50 eV – 200 keV

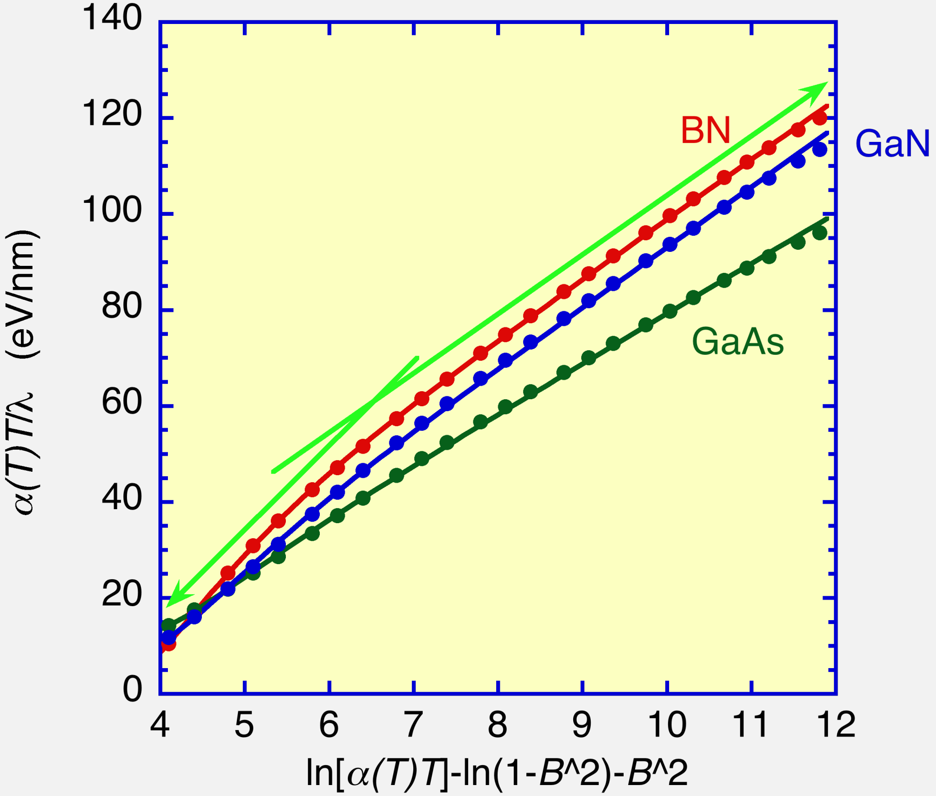
RMS differences (%)

Li	: 0.43
Al	: 0.98
Au	: 0.59

Average of RMS (%) for 41 elemental solids
0.82% (0.4 – 1.4 %)

$$\frac{\alpha(T)T}{\lambda} = E_p^{\ 2}\left\{\beta\left[\ln\left(\gamma\alpha(T)T\right) - \ln\left(1-B^2\right) - B^2\right] - C/T + D/T^2\right\} \quad \text{(nm/eV)}$$

Fano plots and Curve fits for 3 semiconductiors



Solid circles: calculated from IMFPs (rel. FPA method)

Solid lines: Fit with Rel. mod. Bethe equation

Energy range: 50 eV – 200 keV

RMS differnces (%)

BN : 0.58

GaN : 1.1

GaAs : 1.1

Average of RMS (%) for 30 compounds

0.74 % (0.4 – 1.1 %)

$$\frac{\alpha(T)T}{\lambda} = E_p^{\,2}\left\{\beta\left[\ln\left(\gamma\alpha(T)T\right) - \ln\left(1 - B^2\right) - B^2\right] - C/T + D/T^2\right\} \quad \text{(nm/eV)}$$

Relativistic TPP-2M equation

$$\lambda = \frac{\alpha(T)T}{E_p^{\ 2}\left\{\beta\left[\ln\left(\gamma\alpha(T)T\right) - \ln\left(1-B^2\right) - B^2\right] - C/T + D/T^2\right\}} \quad \text{(nm)}$$

$$\beta = -1.0 + 9.44/\left(E_p^2 + E_g^2\right)^{0.5} + 0.69\rho^{0.1} \quad (\text{eV}^{-1}\text{nm}^{-1})$$

$$\gamma = 0.191\rho^{-0.5} \quad (\text{eV}^{-1})$$

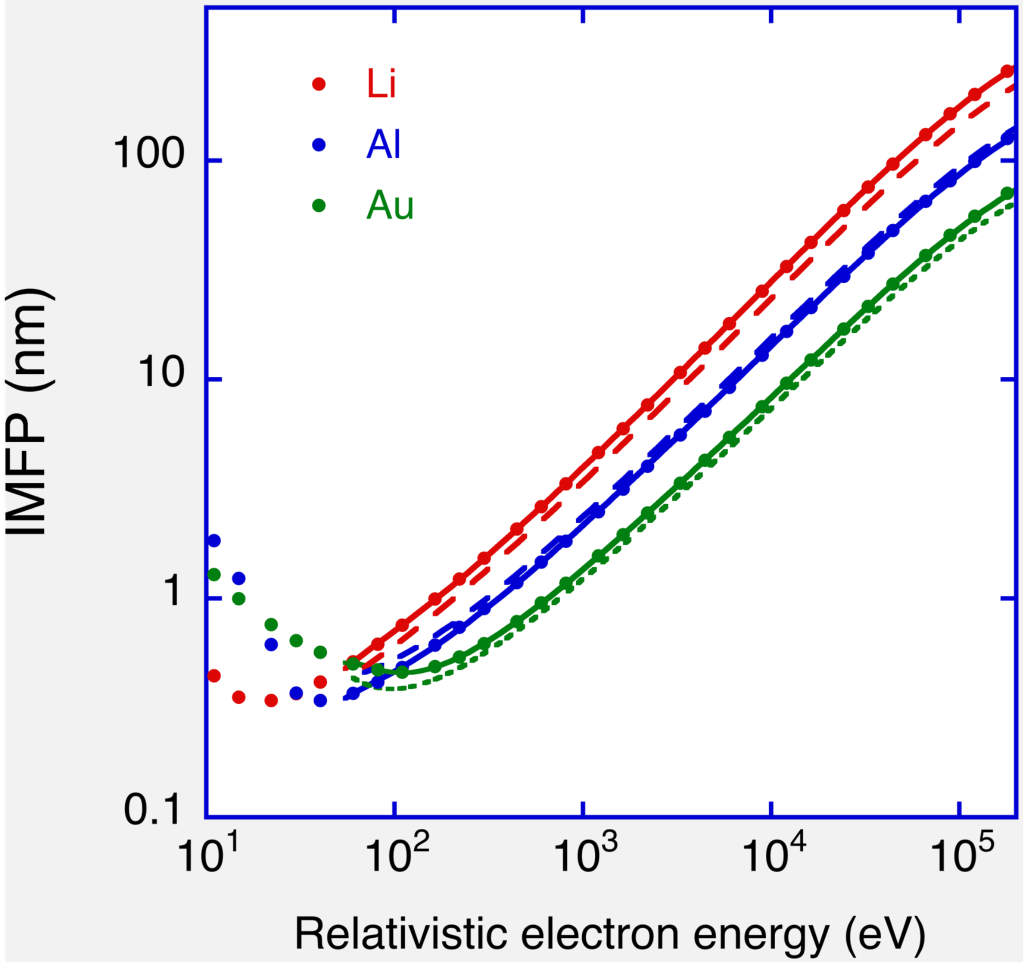
$$C = 19.7 - 9.1U \quad (\text{nm}^{-1})$$

$$D = 534 - 208U \quad (\text{eVnm}^{-1})$$

$$\alpha(T) = \frac{1 + T/\left(2m_ec^2\right)}{\left[1 + T/\left(m_ec^2\right)\right]^2}$$

$$B = \frac{v}{c}$$

Comparison of IMFPs with rel. TPP-2M for 3 elemental solids



Solid circles: calculated with rel. FPA
Solid lines: Fit with Rel. M. Bethe eq.
Dashed lines: rel. TPP-2M

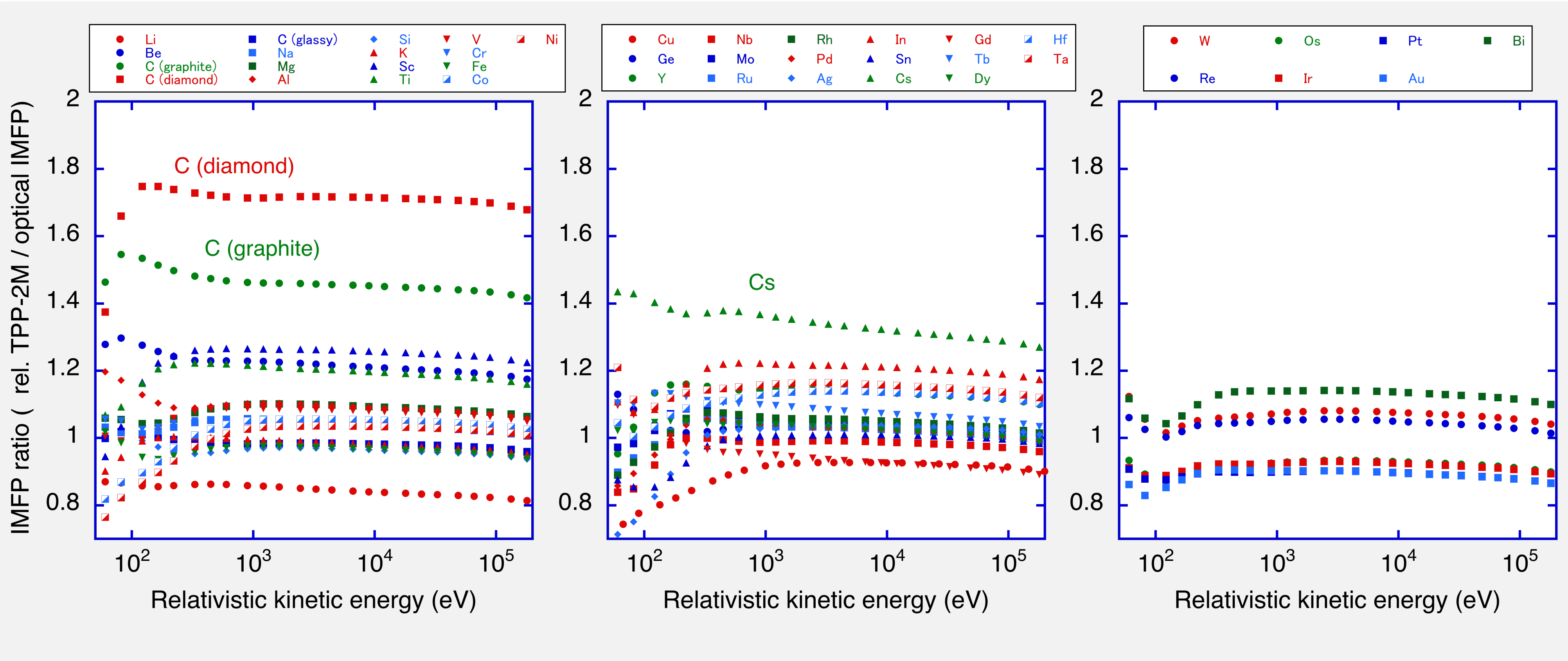
Energy range: 50 eV – 200 keV

RMS differences (%) for rel. TPP-2M

Li	: 15.5
Al	: 10.2
Au	: 11.4

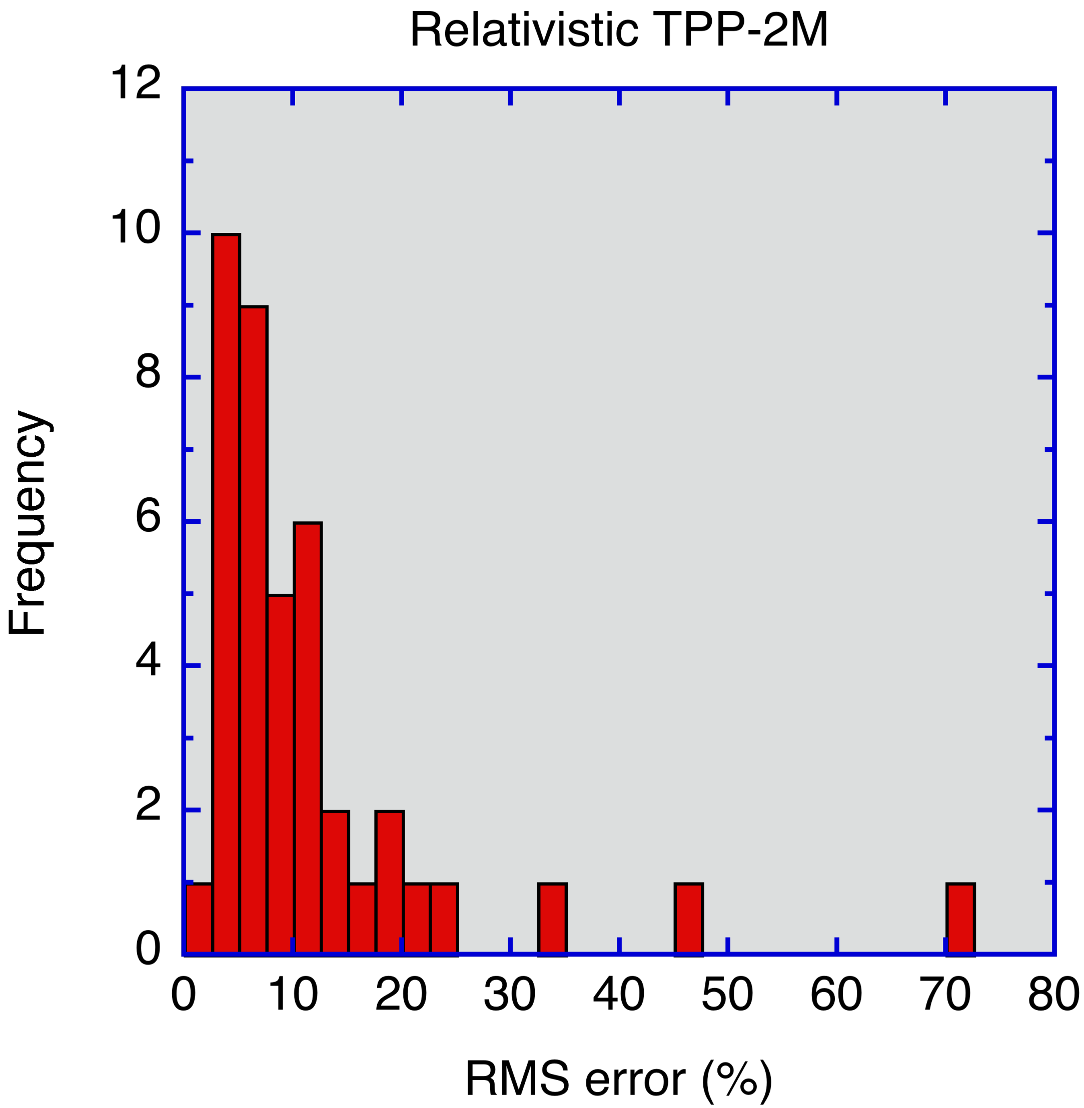
Ratios of IMFPs for 41 elemental solids

IMFP(rel. TPP-2M)/ optical IMFP   vs. electron energy



RMS differences histogram

: energy range 50 eV -200 keV



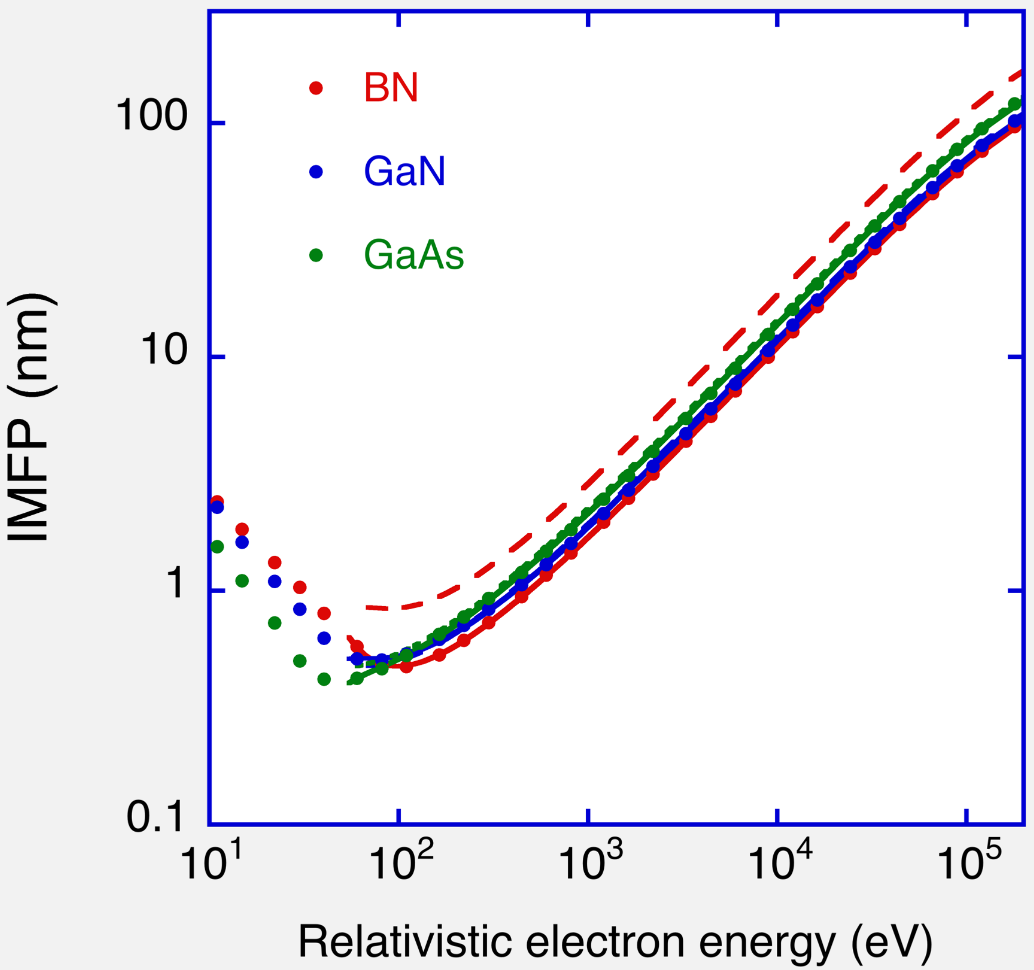
$$RMS = 100 \times \sqrt{\sum_{i=1}^{n} \left(\frac{\lambda_{fit}(E_i) - \lambda(E_i)}{\lambda(E_i)} \right)^2 \Big/ n}$$

Average of RMS (%) for 41 elemental solids

→ 11.9 %

→ 8.9 % (except for diamond, graphite, Cs)

Comparison of IMFPs with rel TPP-2M for 3 compounds



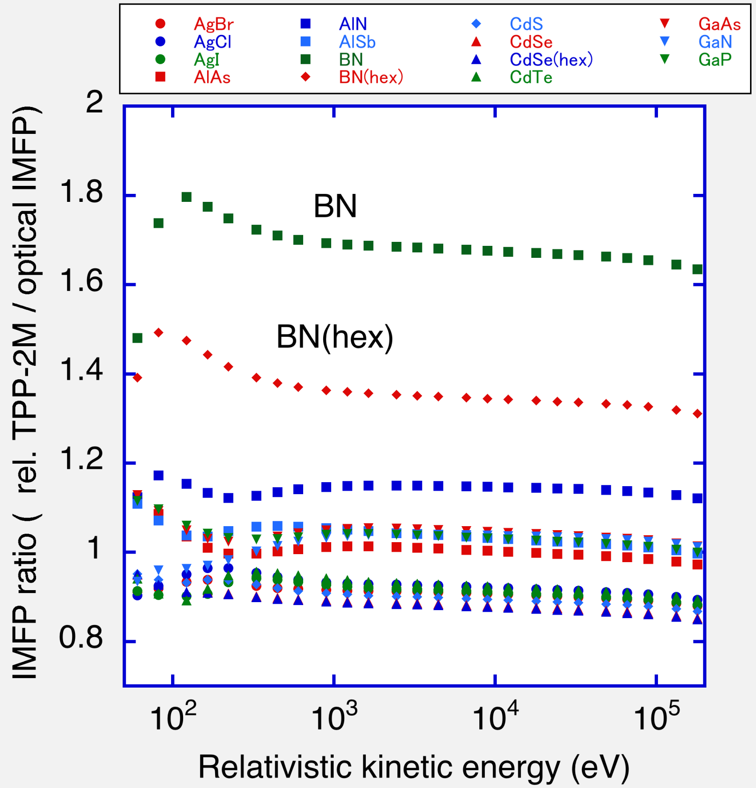
Solid circles: calculated with rel. FPA
Solid lines: Fit with Rel. M. Bethe eq.
Dotted lines: rel. TPP-2M

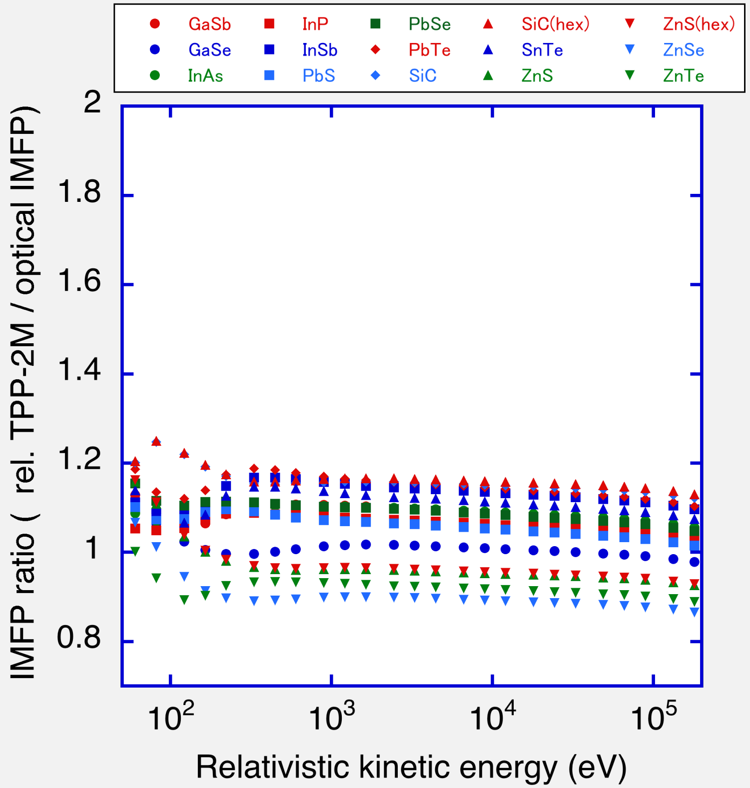
Energy range: 50 eV – 200 keV

RMS differences (%) for rel. TPP-2M

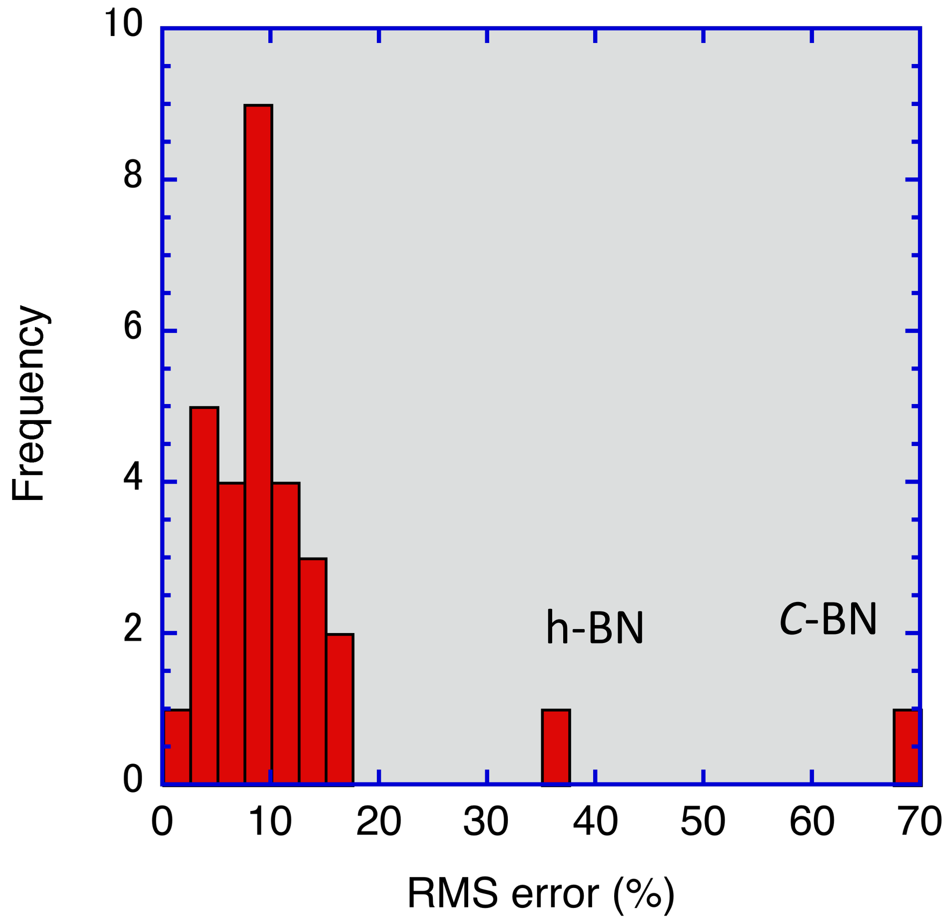
BN	:	68.6
GaN	:	3.4
GaAs	:	5.0

Ratios of IMFPs for 30 compound semiconductors





RMS differences histogram for compounds
: energy range 50 eV -200 keV



Average of RMS (%) for 30 compound semiconductors
11.7 % (2.4 – 69 %)

8.8 % (except BN)

Electron exchange effect on IMFP calculation

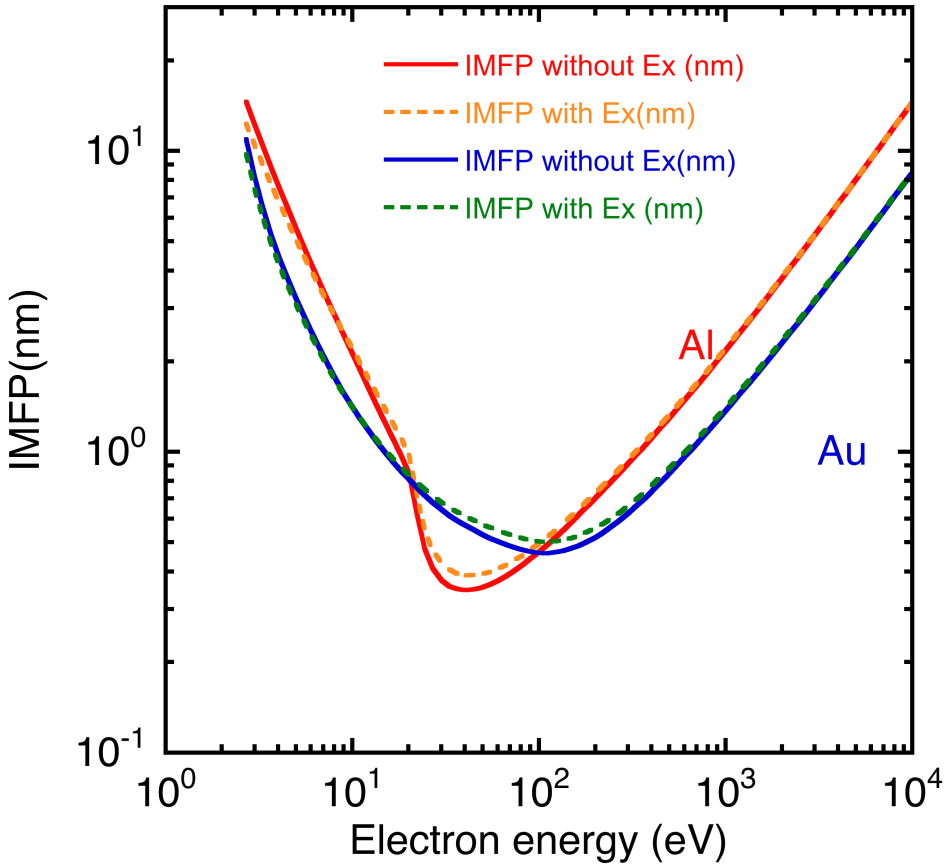
- important to know the effect of exchange between projectile and target electrons on IMFP calculations with the FPA.
- no consensus on how to incorporate exchange effects within the dielectric formalism
- estimate the influence of electron exchange on IMFPs using the Born-Ochkur exchange correction.

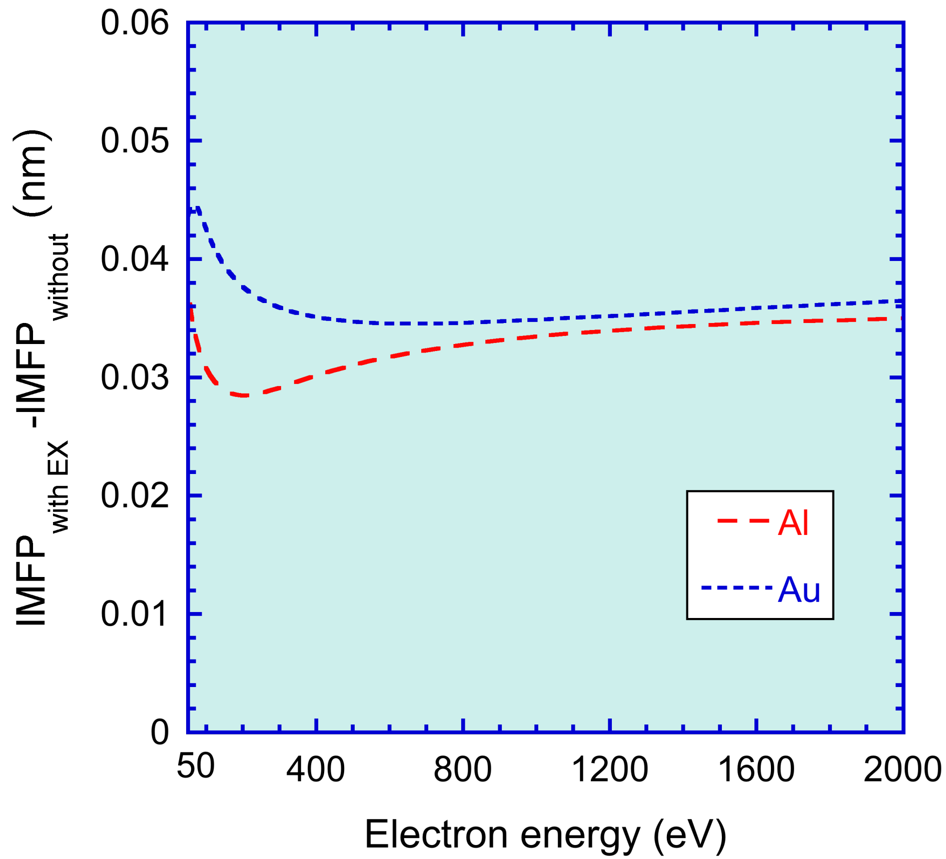
The non-relativistic DCS with the Born-Ochkur correction can be written as (Fernandez-Varea *et al*.)

$$\frac{d^2\sigma}{dq\,d\omega} = \left(1 - \frac{q^2}{2E} + \left(\frac{q^2}{2E}\right)^2\right) \frac{1}{\pi N E} \operatorname{Im}\left[\frac{-1}{\varepsilon(q,\omega)}\right] \frac{1}{q}$$

-calculated IMFPs of **Al, Si, Cu, Ag, and Au** with and without the exchange correction and compared them.

Influence of electron exchange on IMFPs

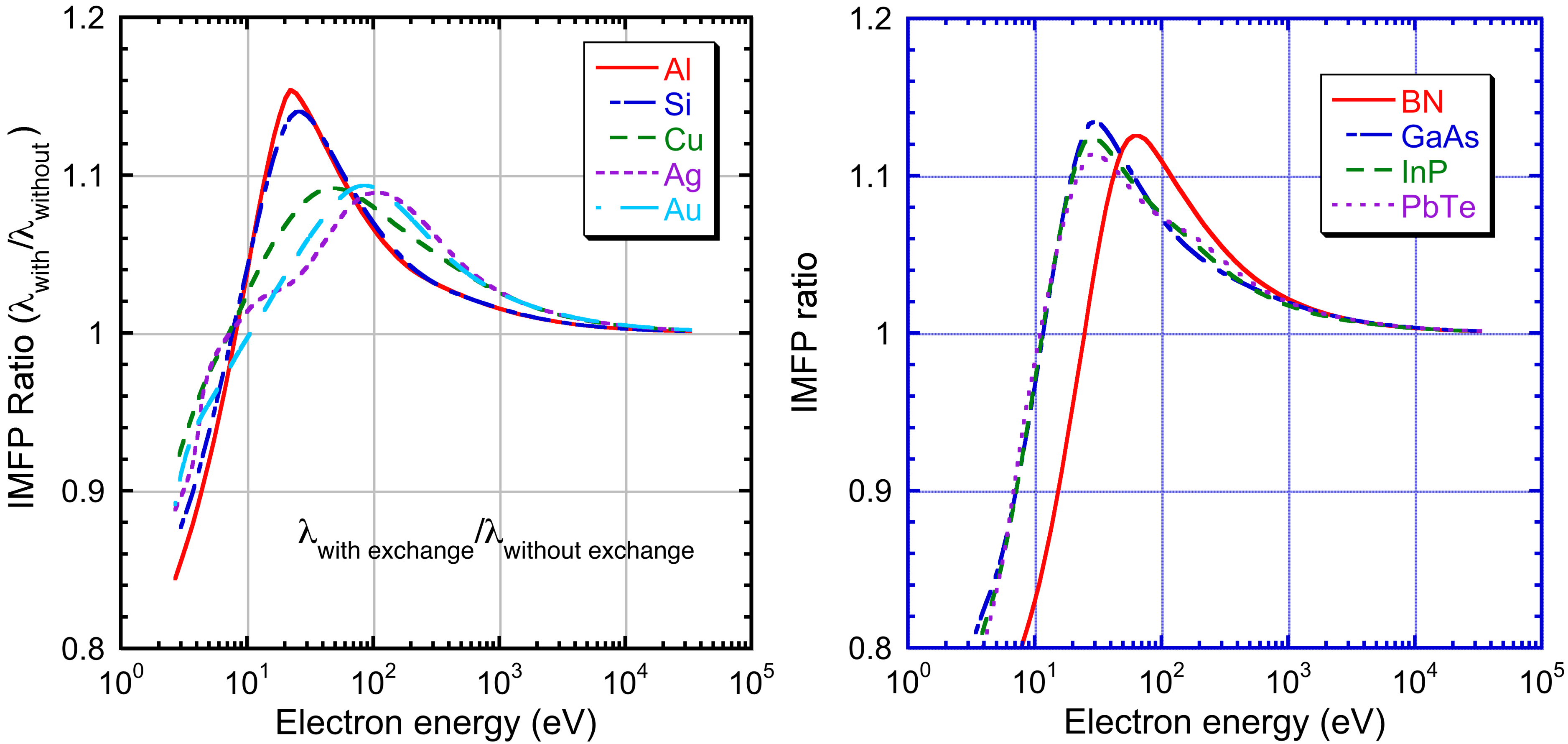




- IMFPs with the exchange correction are larger than those without the exchange correction for Al and Au between 50 eV and 30 000 eV.

- Above 50 eV, the difference between IMFPs with and without exchange correction are less than 0.05 nm for these elemental solids.

Influence of electron exchange on IMFPs



- Above 100 eV, the difference between IMFPs with and without exchange correction are less than about 10% for these elemental solids.

- Born-Ochkur corr. is essentially a high-energy approximation. It is then not clear whether this approximation is useful for evaluating the exchange correction for energies less than 100 eV.

Comparison of Mermin model for IMFPs

-Denton *et al. (SIA 2008,p1481)* reported IMFP calculations for Al and Au that were based on the use of a Mermin ELF function.
The Mermin function is an improvement over the Lindhard dielectric function utilized in the Penn algorithm in that it accounts for the finite lifetimes of the various excitations.

- De la Cruz and Yubelo also calculated IMFPs of Si, Ti, Ag, and Au for 200 – 20 000 eV using similar Mermin ELF function.

- They compared their IMFPs to the IMFPs calculated by SPA (with quadratic dispersion eq.).
Then, we have compared their Mermin model with our Penn model : FPA and SPA (with quartic dispersion eq.)

Mermin ELF model

- Denton approach (MELF-GOS model)

  - energy dependence q=0 : Drude function (fit to optical ELF)

$$q = 0 \quad \varepsilon^M\left(q = 0, \omega; \omega_p; \gamma\right) = 1 - \frac{\omega_p^2}{\omega(\omega + i\gamma)} = \varepsilon^D\left(\omega; \omega_p; \gamma\right)$$

Drude type DF

$$\mathrm{Im}\left[\frac{-1}{\varepsilon_M\left(q = 0, \omega\right)}\right]_{outer} = \sum_i A_i \,\mathrm{Im}\left[\frac{-1}{\varepsilon_D\left(q = 0, \omega; \omega_{p,i}, \gamma_i\right)}\right]$$

parameters: relative weight, position, and width

ε_D : Drude type ELF

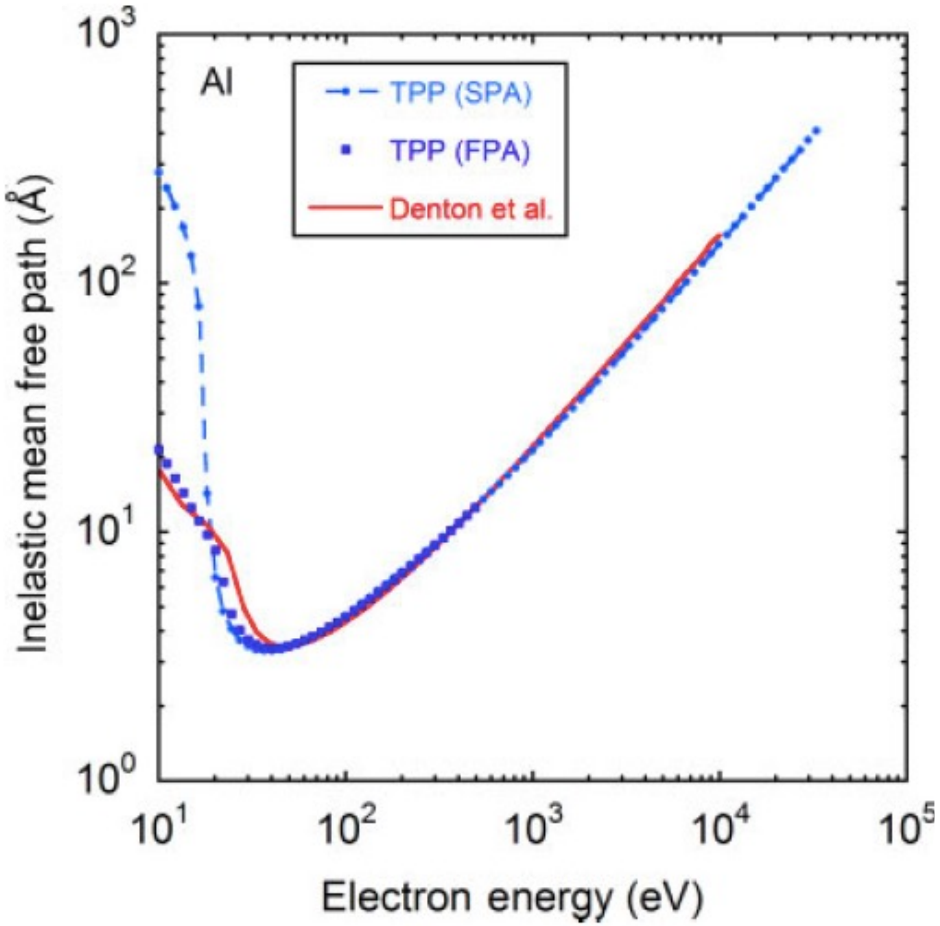
- q dependence (q>0)

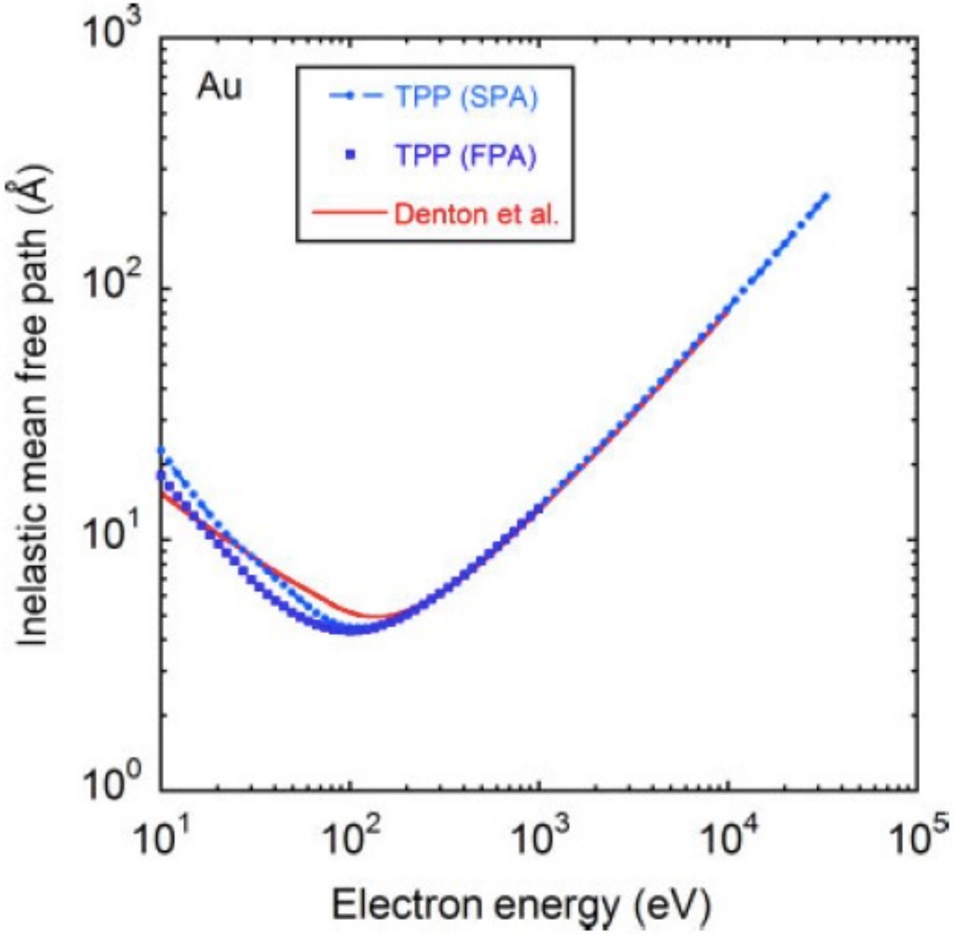
$$\varepsilon_M\left(q, \omega\right) = 1 + \frac{1 + i\gamma / \omega}{\left[\varepsilon_L\left(q, \omega + i\gamma\right) - 1\right]^{-1} + \left(i\gamma / \omega\right)\left[\varepsilon_L\left(q, 0\right) - 1\right]^{-1}}$$

$$\gamma = 0 \quad \varepsilon^M\left(q, \omega; \omega_p; \gamma \to 0\right) \to \varepsilon^L\left(q, \omega; \omega_p\right)$$

Lindhard DF (limiting form)

Comparisons of IMFPs : Al and Au

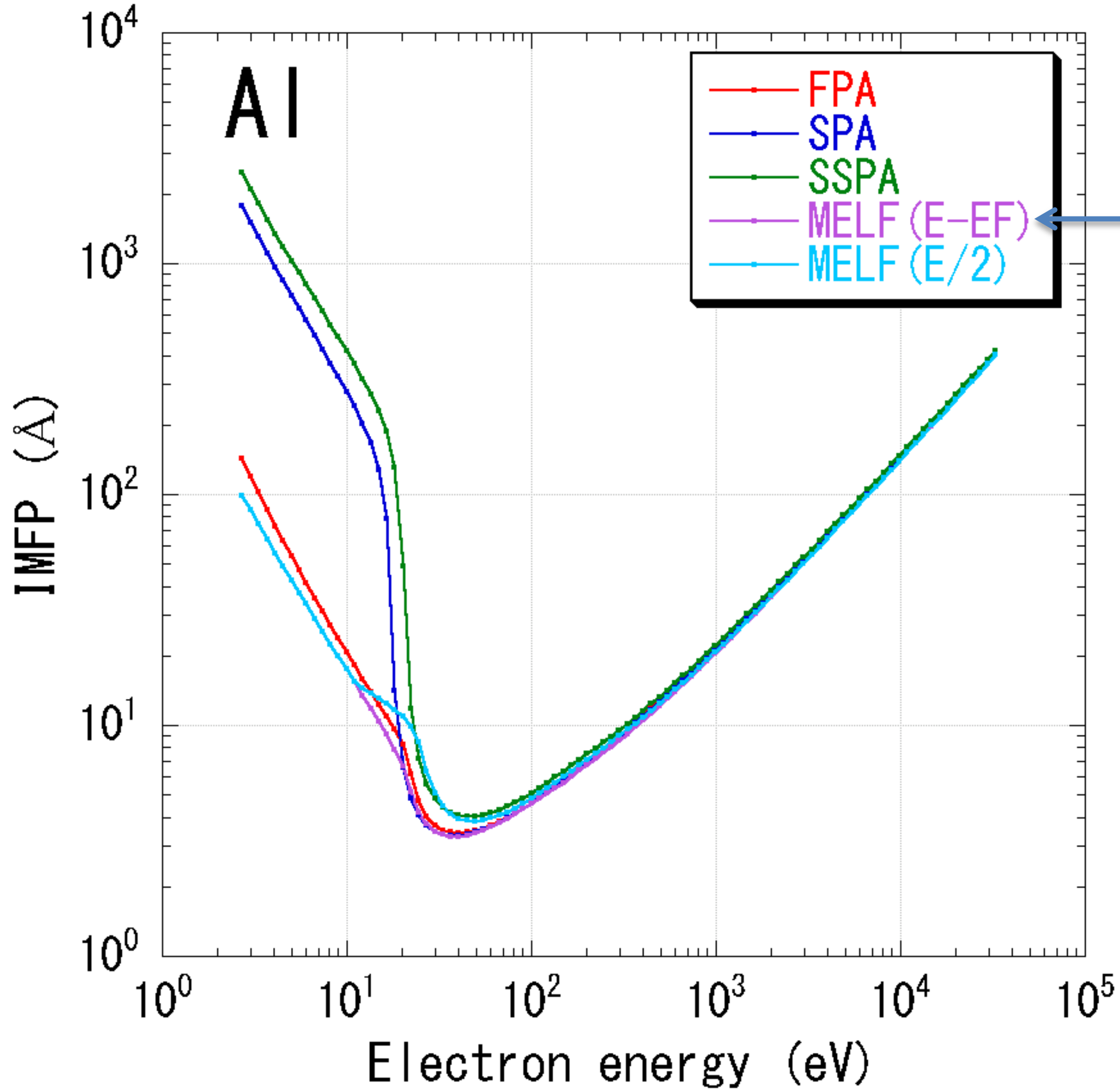




ω_{max} = E – E_f for TPP
ω_{max} = min [E/2 , E – E_f] for Denton et al.

$$\lambda = \left[\int_0^{\omega_{max}} p(E,\omega)\, d\omega \right]^{-1}$$

Comparisons of IMFPs : Al



$\omega_{max} = E - E_f$

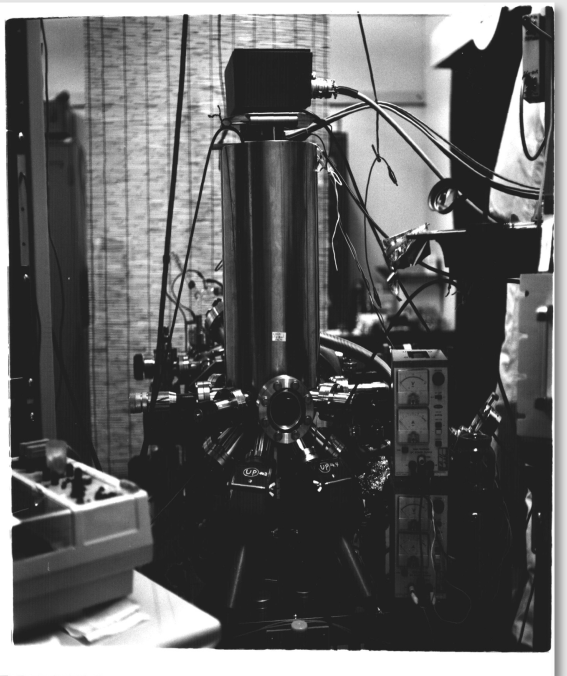
4. Comparison of IMFPs from EPES experiments

: to know the reliability of IMFPs calculated from ELFs with Penn algorithm (optical IMFP) and from TPP-2M.

-determine IMFPs for Ag, Au, Cr, Cu, Fe, Ga, C (Graphite) , Mo, Pt, Si, Ta, W and Zn in the 50 - 5000 eV energy range from backscattered elastic-peak intensities (EPIs) using Ni-reference

-compare with the corresponding calculated IMFPs (optical and TPP-2M).

Measurements of EPIs by absolute CMA



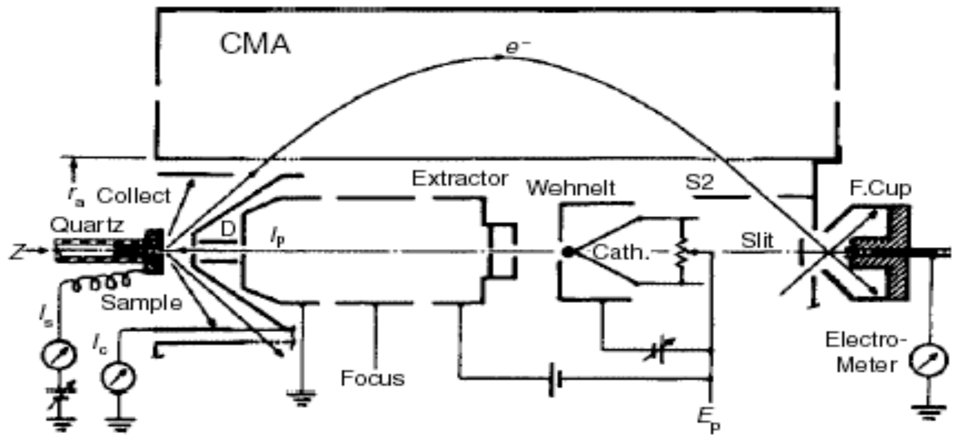


Figure 1. Schematic CMA system.

CMA ΔE/E = 0.25%

Accuracy

± 0.01% (primary beam energy)

± 0.5% (Auger spectra)

Measurement of Elastic Peak Intensity
Energy range : 1 - 5,000 eV
(50 - 5,000 eV)
Instrument: Absolute Auger Spectrometer
-detection angle (42.3± 6°)

Primary beam: 1μA
Detector: Faraday cup

Calculation of EPI with MC method

$$I = G_t \times f_s \times \int_0^\infty \left(\frac{d\eta}{dS}\right)/N_0 \exp\left(-\frac{S}{\lambda}\right) dS$$

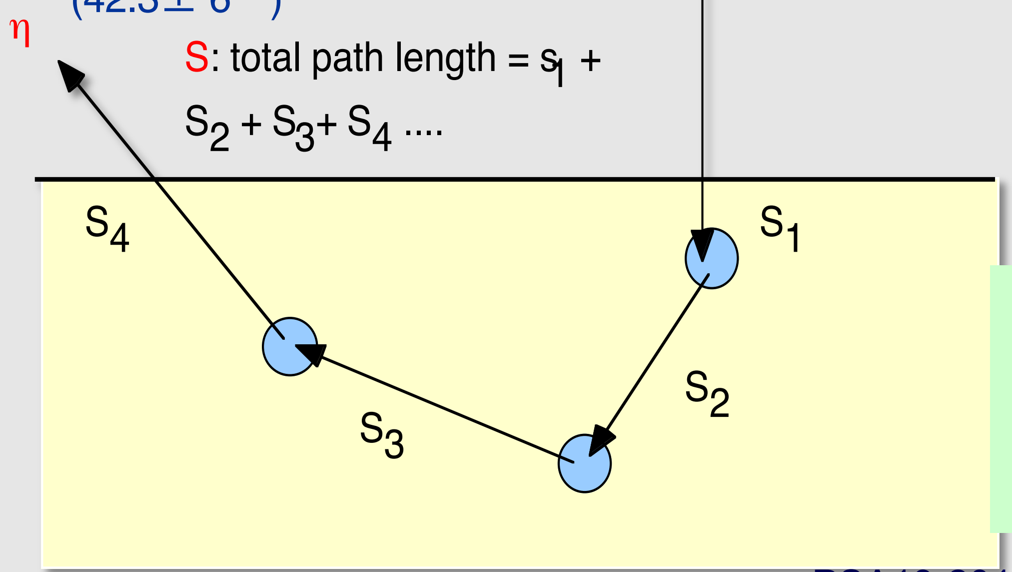
Surface excitation factor

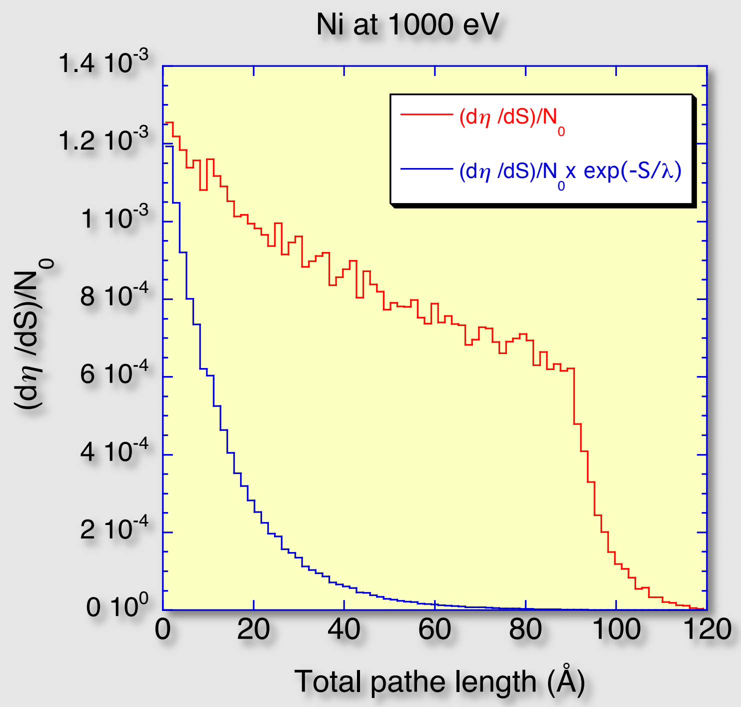
path-length distribution of electrons detected by CMA (42.3± 6°)

IMFP

e^-

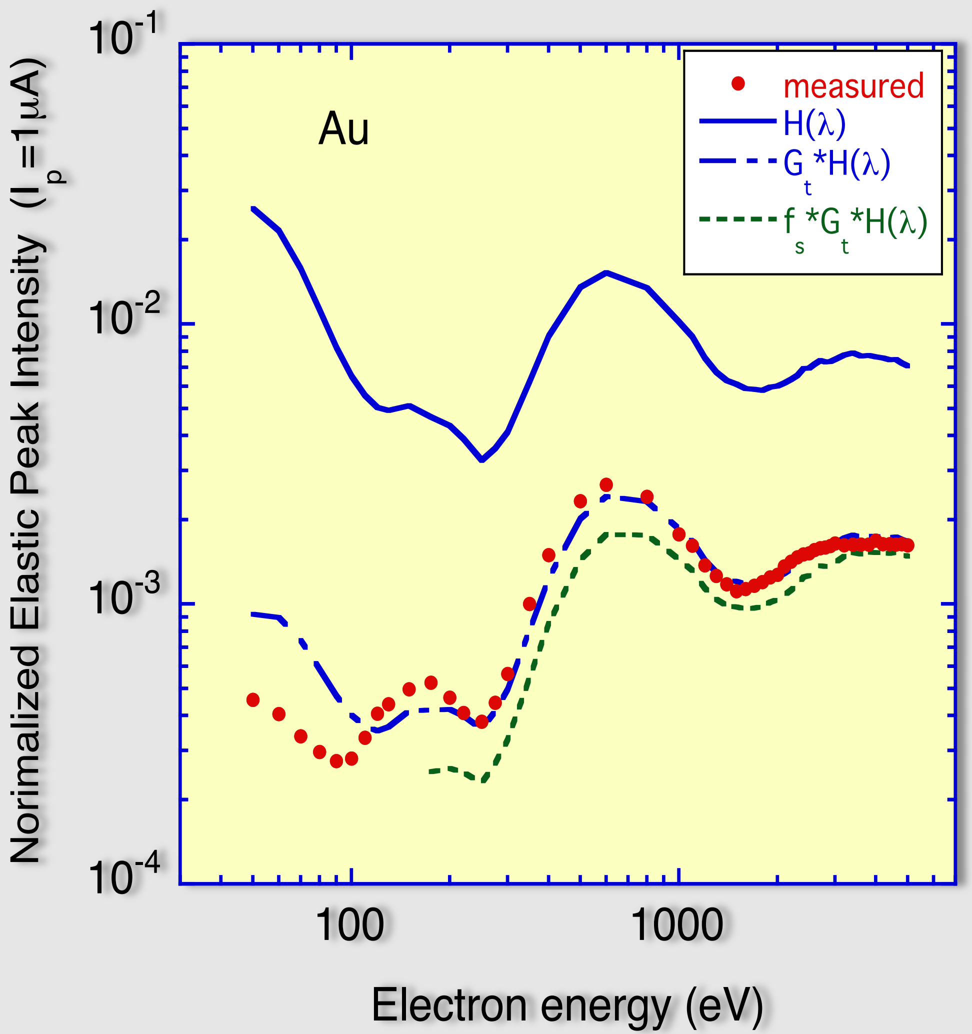
S: total path length = s_1 + S_2 + S_3 + S_4 ....





:Elastic scattering cross section
TFD potential
: Pseudo random number generator
Mersenne Twister

EPIs for Au in the 50 - 5000 eV



$$\left(\frac{I^x}{I_0}\right)_{cal} = G_t f_S \int_0^\infty (d\eta/dS)^x / N_0 \exp(-S/\lambda_x)\, dS$$

$$= G_t f_S H(\lambda)$$

Measured intensity
- solid circles: EP current /incident

Calculated intensities from MC method
H (λ) - solid line (optical IMFPs)
Gt* H(λ) - long dash line
Gt*fs*H(λ) - short dash line
fs : Werner et al., Surf. Sci. 2001; 486: L461.

$$G_t \ll f_s \leq 1$$

uncertainty of G_t : ?

200eV > : good agreement

200 eV< : large difference

Determination of IMFPs using Ni reference

Determination of IMFPs from EPIs using Ni-std **; remove G_t**

$f_s^x / f_s^{Ni} = 1$ - assume that surface excitation effect is negligible for Ni-reference method.

$$\left(\frac{I^x}{I^{Ni}}\right)_{cal} = \frac{\int_0^\infty (d\eta/dS)^x / N_0^x \exp(-S/\lambda_x) dS}{\int_0^\infty (d\eta/dS)^{Ni} / N_0^{Ni} \exp(-S/\lambda_{Ni}) dS}$$

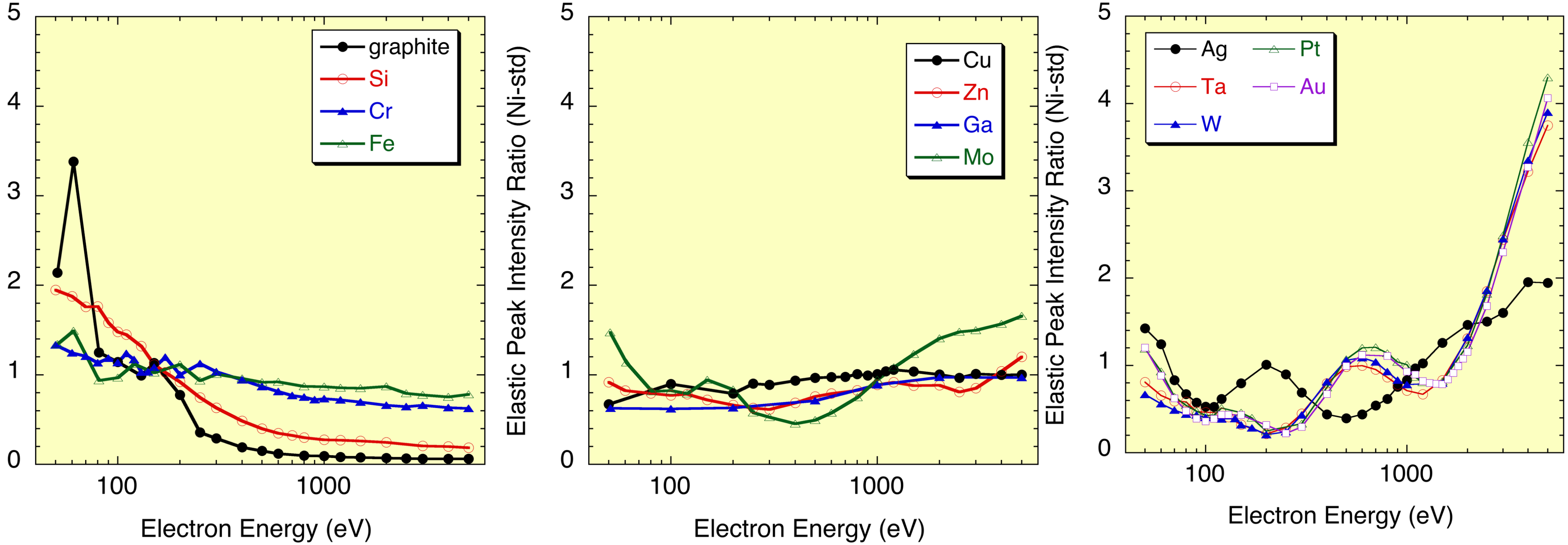
: Determination of IMFPs using Ni-std

Then,

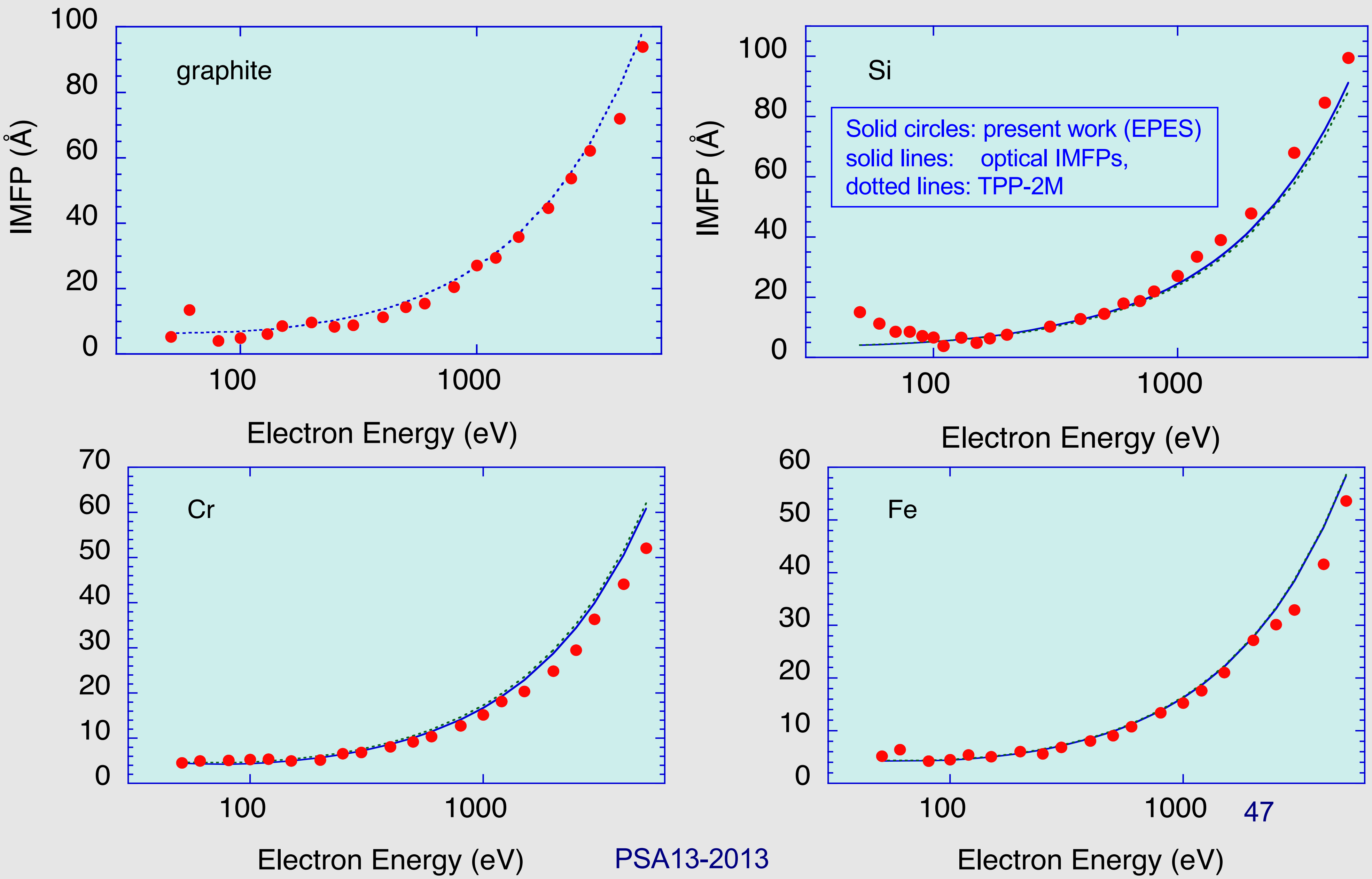
$$\left[\left(\frac{I^x}{I^{Ni}}\right)_{mesaured} - \left(\frac{I^x}{I^{Ni}}\right)_{cal}\right]^2 \rightarrow min$$

- solve above eq. for parameter λ_x (IMFP) for the target material (with solver in Excel)

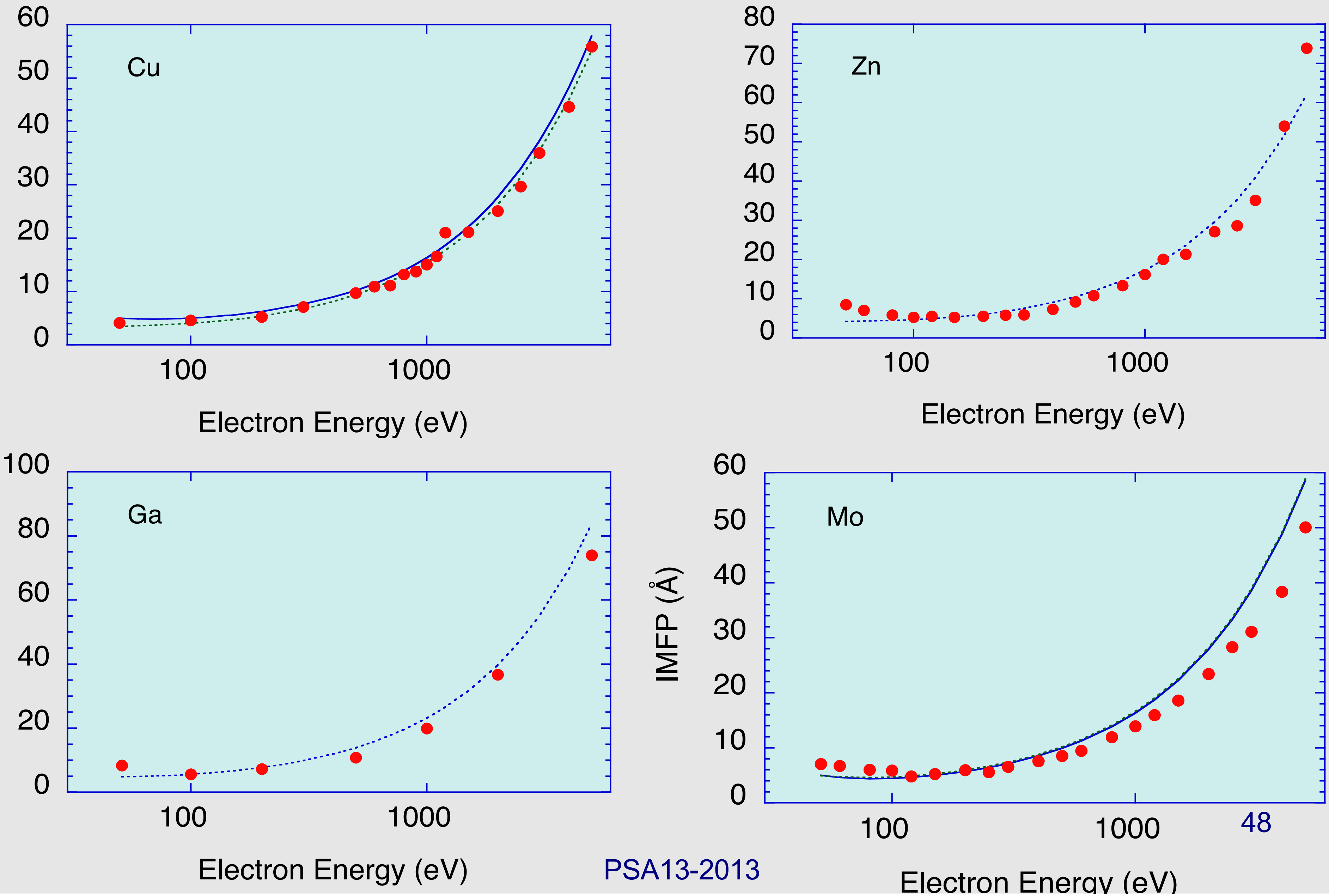
Measured elastic peak intensity ratios (Ni-std) as a function of electron energy



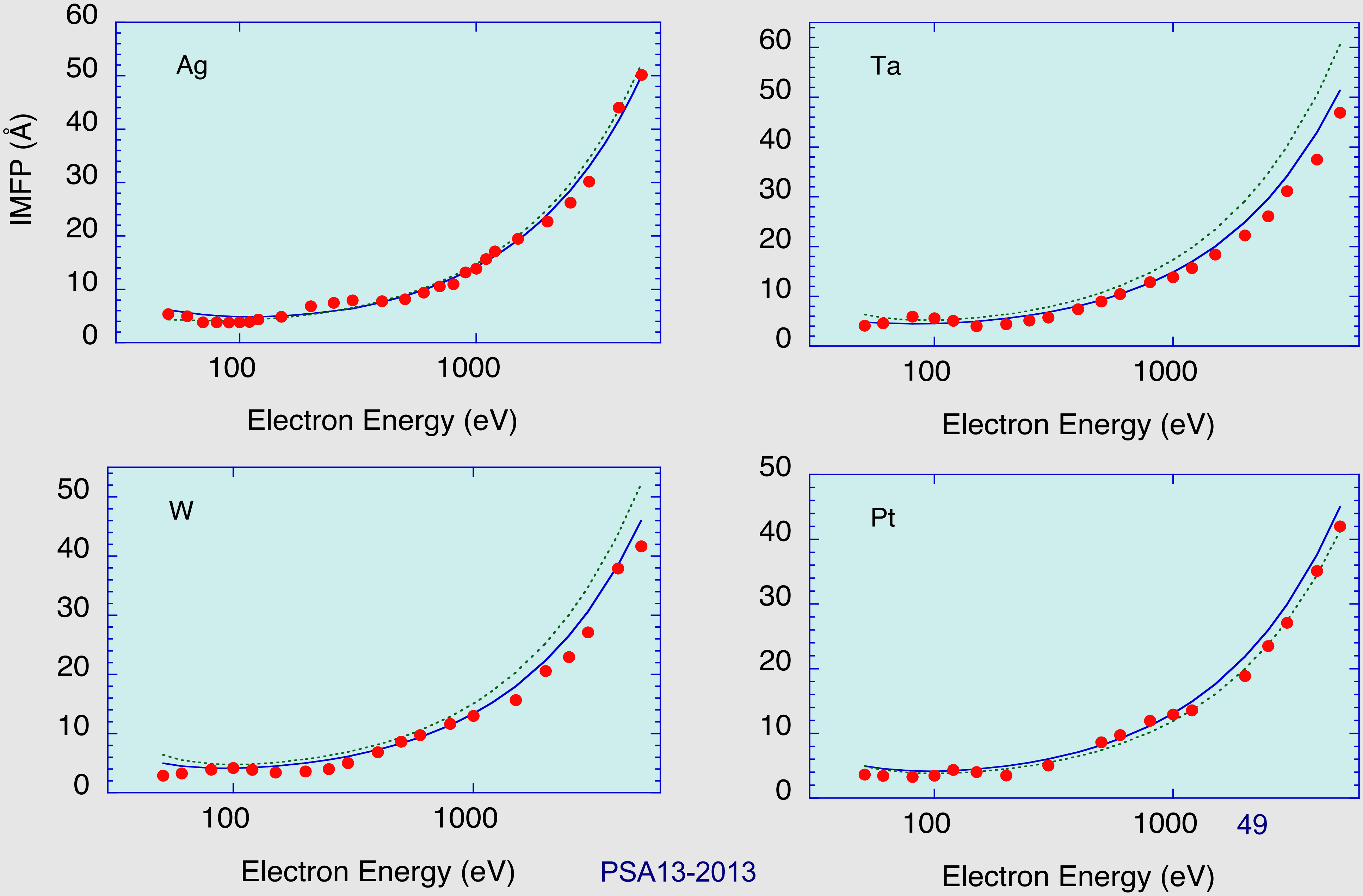
IMFPs determined from EPI ratios



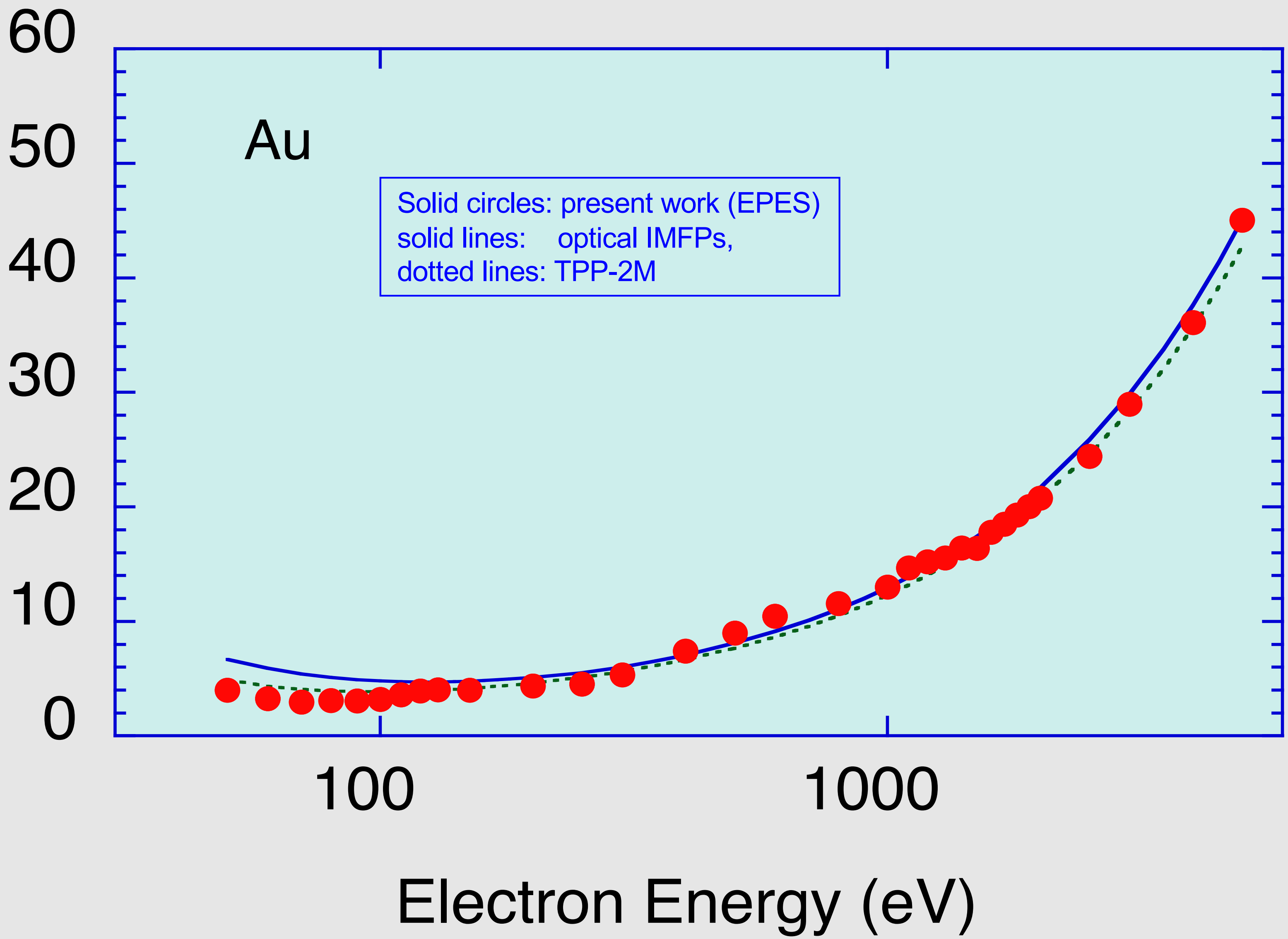
IMFPs determined from EPI ratios for Cr, Fe, Ga and Graphite



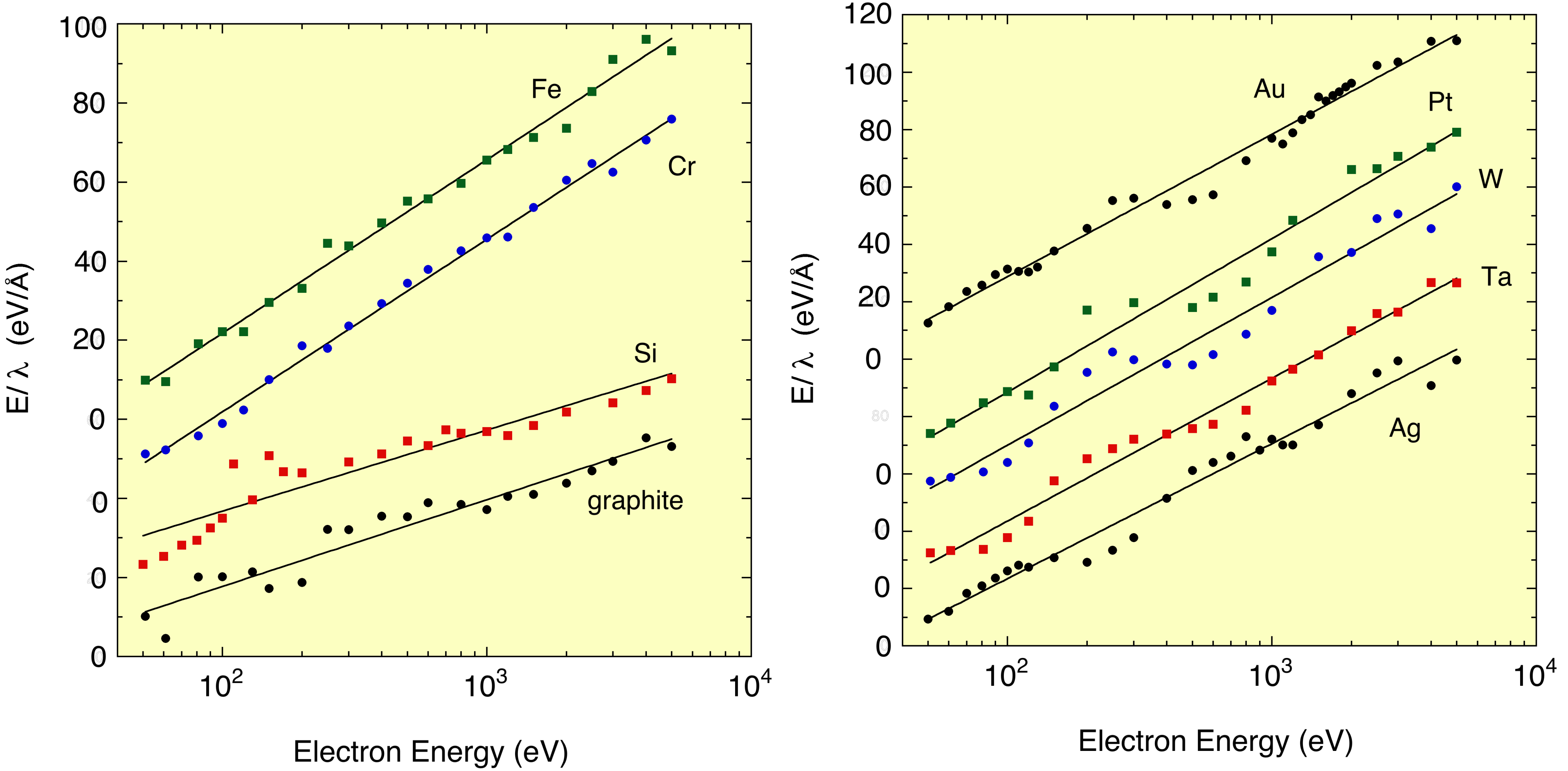
IMFPs determined from EPI ratios for Cr, Fe, Ga and Graphite



IMFPs determined from EPI ratios for Au,Ag,Cu, Si



Analysis of IMFPs with Fano Plot



$$E/\lambda = E_p^2\,\beta \ln(\gamma E)$$

Simple Bethe equation

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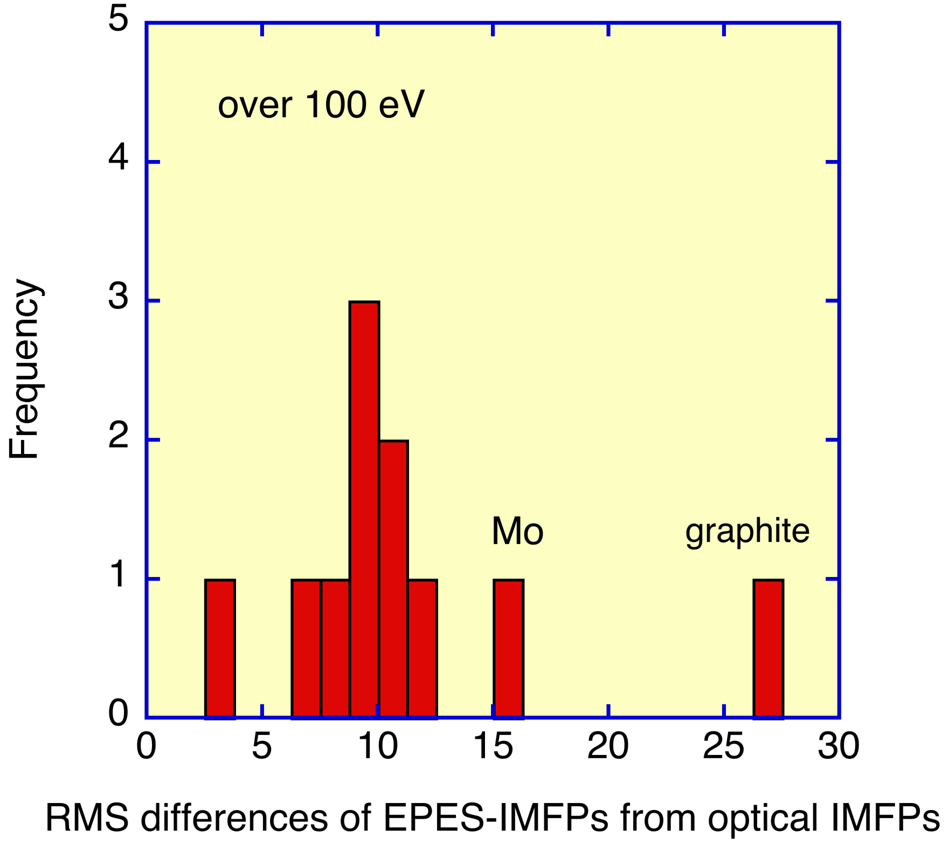
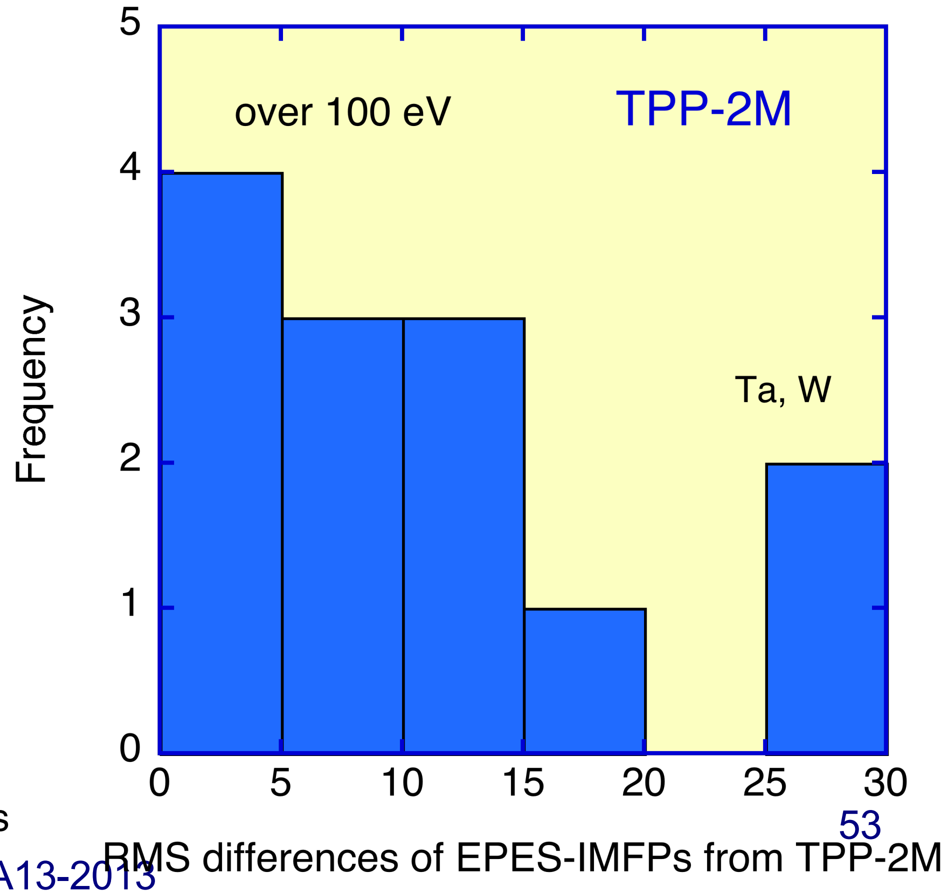
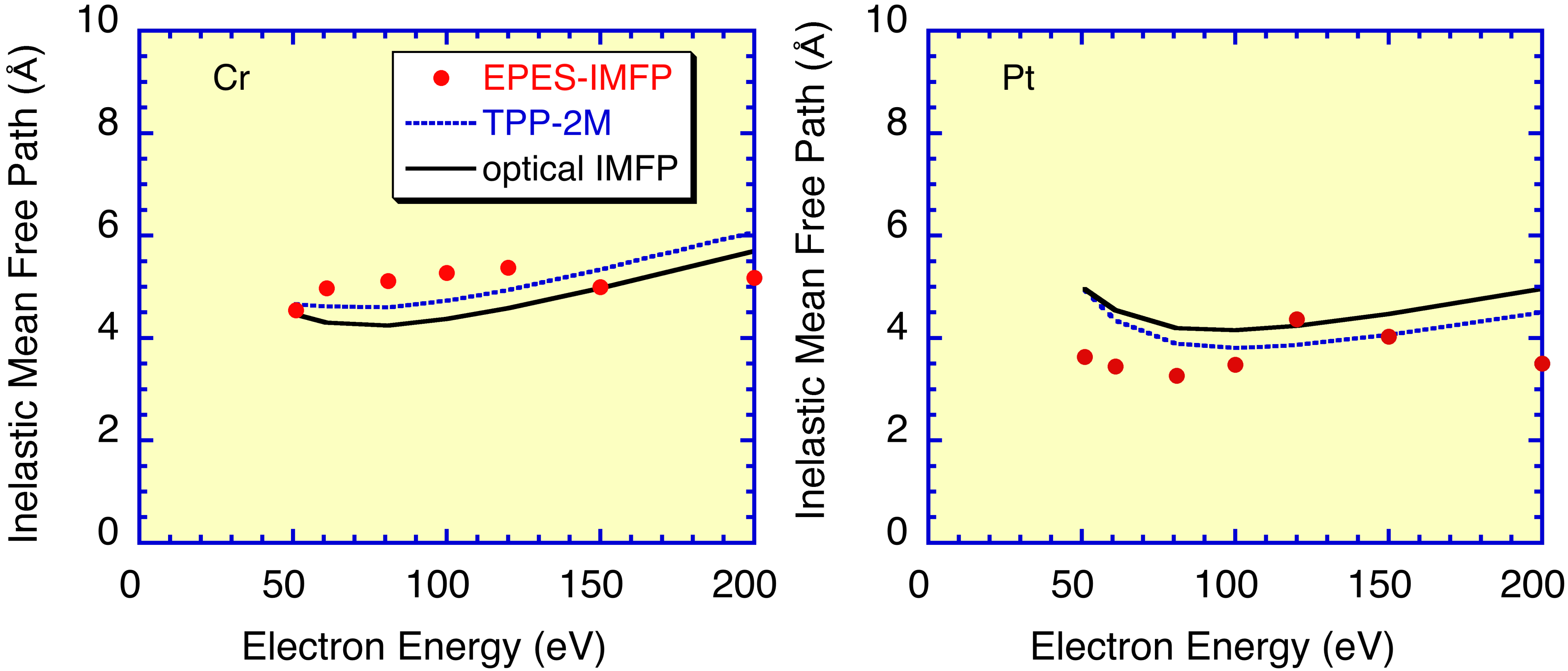
RMS (%) difference of IMFPs
- IMFPs of the Penn algorithm (optical IMFPs) and the TPP-2M

Average RMS(%) in 100 - 5000 eV : 11.0%(optical)
10.7%(TPP-2M)



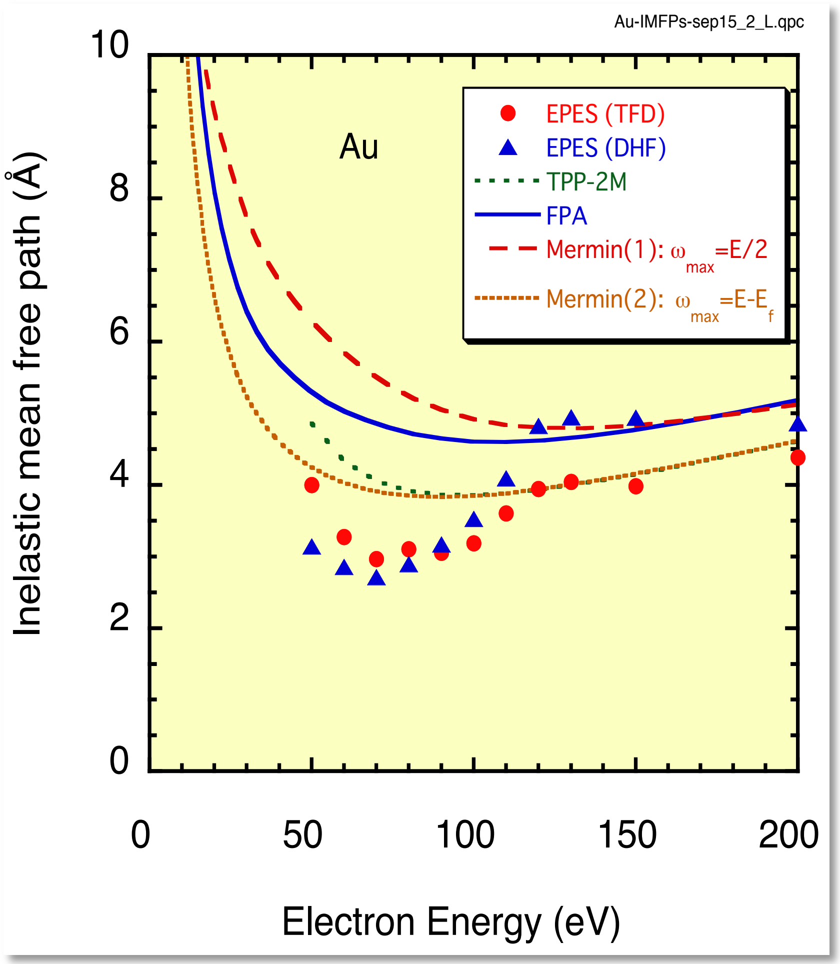


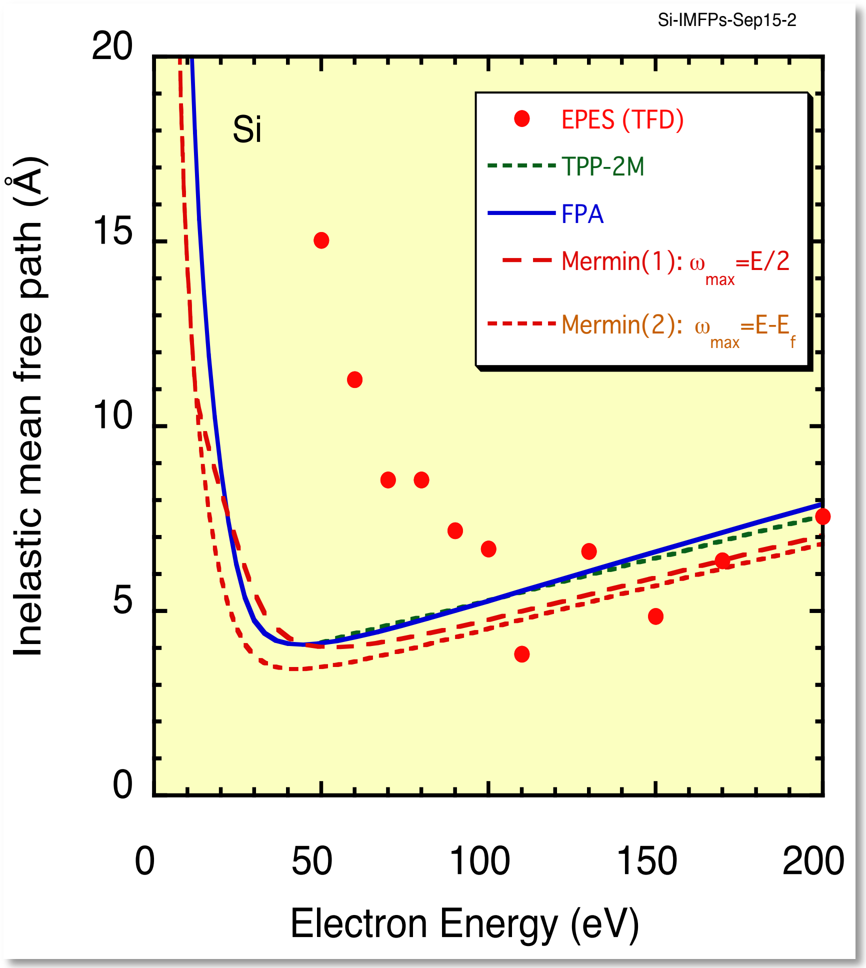
Comparison of IMFPs from EPES experiments at low energy region **(under 200 eV)**



* almost same results for Ag, Cu, Fe, Ta and W

Comparison of IMFPs from EPES experiments at low energy region (under 200 eV)





* surface excitation effect for EPES
* electron exchange effect , correlation effect
* IMFP values of Ni STD at low energy

5. Summary

- We calculated IMFPs for 41 elemental solids and 30 compound semiconductors from experimental and calculated optical data for electron energies from 10 eV to 200 keV using relativistic FPA

- Relativistic Modified Bethe equation fits optical IMFPs well over 50 eV – 200 keV. Average RMS : 0.8% for elemental solids, 0.7% for semiconductors.

- Relativistic TPP-2M equation provides reasonable estimates of IMFPs over 50 eV – 200 keV.
  Average RMS : < 12% in both group.
  : down to < 9% (except for graphite, diamond, Cs and BN)

5. Summary -2

- We also carried out the experimental determinations of IMFPs for 13 elemental solids in the 50-5000 eV energy range from backscattered EPIs using a Ni reference together with MC.

- The IMFPs determined from EPES could be fit by a simple Bethe formula in the 100 – 5000 eV energy range using Fano plot (average RMS deviation : 9%)

- The EPES-IMFPs of Ag, Au, Cr, Cu, Fe, Pt, Si, Ta and W are in excellent agreement (**RMS deviations is less than 11%**) with those calculated from the Penn algorithm (optical IMFPs) in the 100-5000 eV energy range.

These works were performed in collaboration with

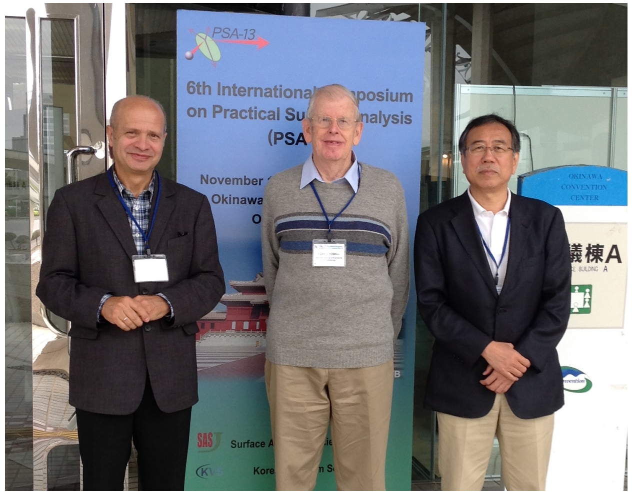
C. J. Powell, D. R. Penn (NIST) : IMFP calculations

H. Shinotsuka (NIST, AA&S) : OCs and programing

K. Goto (NIT, AIST) : EPI measurements

Jun. 1987

Nov. 2004



Nov. 2013

Thank you for your attention !