Inelastic Mean Free Paths, Mean Escape Depths, and Effective Attenuation Lengths for Surface Electron Spectroscopies

S. Tanuma,[1] K. Goto, [2] H. Yoshikawa,[1] C. J. Powell,[3]
D.R. Penn[3,] B. Da,[1] R. Ueda,[1] and H. Shinotuka[1]
(*1:NIMS , 2:AIST 3: NIST)*

1. Parameters used for describing the attenuation of signal electrons
   : definitions of IMFP, EAL, MED
2. Calculations of IMFPs in solids
   : 41 elemental solids and 31 inorganic compounds.
3. Measurements of IMFPs in solids
   : EPES 10 eV – 5 keV
4. IMFPs and EALs in liquid water
   : evaluation of ELF at q>0
5. MEDs for practical SR-XPS
6. Summary

1. Introduction : Definitions of parameters for attenuation of signal electrons

- Parameters for signal electron attenuation in solids

  - inelastic mean free path (IMFP) : nm

  → **Bulk quantity** (fundamental)

  - mean escape depth (MED) : nm (surface sensitivity)
  - effective attenuation length (EAL) : nm (thickness determination)
  - information depth (ID) : nm

  → **From IMFPs**
  experimental conditions ; probe , emission angle, etc)

calculated from emission depth distribution function (EDDF)
: escape probability of signal electrons emitted at depth z

- SLA: (ignore the elastic scattering)
  IMFP = EAL = MED (at θ=0)
- *Practical*
  → IMFP ≠ EAL ≠ MED (θ=0)

IMFP: inelastic mean free paths

Definition: ISO18115-1 (2013)

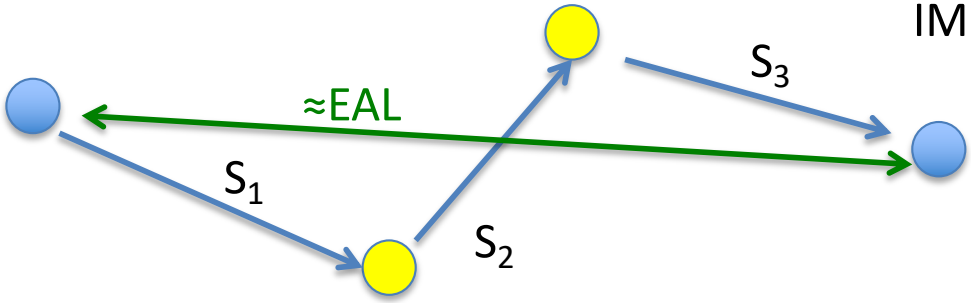
- average distance that an electron with a given energy travels between successive inelastic collisions

- most basic material parameter for describing the surface sensitivity (and/or matrix effect) for AES, XPS and other surface electron spectroscopies.
- EAL, MED can be calculated from IMFPs

Inelastic scattering

Elastic scattering

$IMFP = S_0$



$IMFP = S_1 + S_2 + S_3$

(normally) $IMFP \geq EAL$

Probability : $\exp(-S/\lambda)$

- when $S_0 = S_1 + S_2 + S_3$ ⇒ Same Probability

EAL: effective attenuation length ISO18115-1

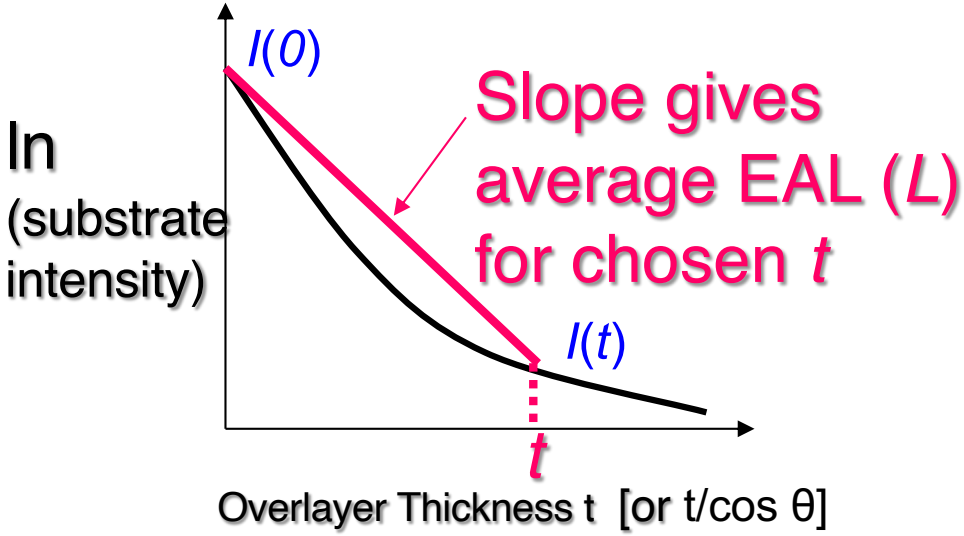
Definition of EAL: parameter which, when introduced in place of the IMFP into an expression derived for AES and XPS on the assumption that elastic-scattering effects are negligible for a given quantitative application, will correct that expression for elastic-scattering effects

Note 1. The EAL may have different values for different quantitative applications of AES and XPS. However, the most common use of EAL is the determination of overlayer-film thicknesses from measurement of the changes in substrate Auger-electron or photoelectron signal intensities after deposition of a film or as a function of emission angle. For emission angles of up to about 60°, it is often satisfactory to use a single value of this parameter. For larger emission angles, the EAL can depend on this angle.

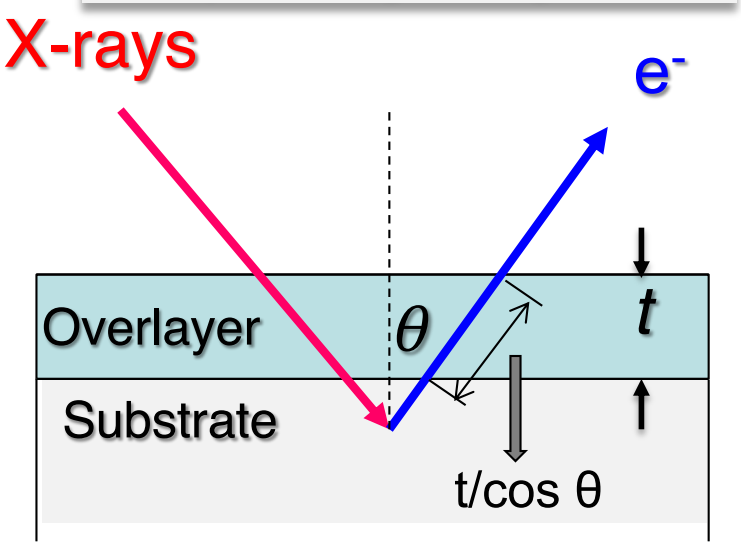
Note 2. Since there are different uses of EAL, it is recommended that users specify clearly the particular application and the definition of the parameter for that application (e.g., by giving an equation or by providing a reference to a particular source).

EAL

- determination of EALs from changes of a substrate XPS peak intensity with overlayer film thickness



Sample-tilting configuration



$$L = \frac{t}{\cos\theta}\frac{1}{\left(\ln I(0) - \ln I(t)\right)}$$

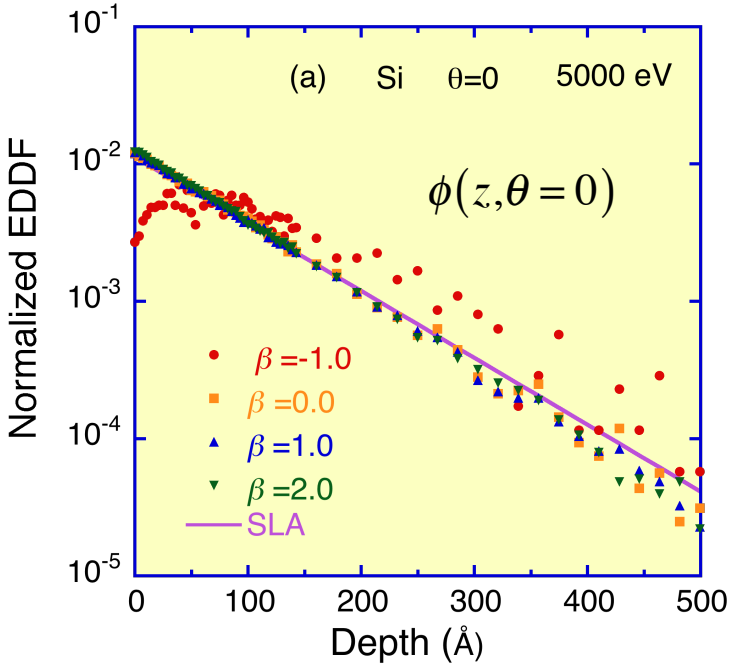
I(0) and *I(t)* are the substrate signal intensities before and after deposition of a film of thickness, *t,* and *θ* is the electron emission angle with respect to the surface normal. The average EAL, *L*, is an empirical parameter for the particular conditions (*t, θ*, and experimental configuration in XPS).

MED mean escape depth

Definition of MED: average depth normal to the surface from which the specified particles or radiation escape as defined by

$$D = \frac{\int_0^\infty z\phi(z,\theta)\,dz}{\int_0^\infty \phi(z,\theta)\,dz}$$

where $\phi(z,\theta)$ is the emission depth distribution function (EDDF) for depth z from the surface into the material and for angle of emission θ with respect to the surface normal.



β: asymmetry parameter

IMFP = EAL = MED (at θ =0) *or*
MED = IMFP x cos θ *when elastic scattering is ignored*

- Practical case MED/cos θ < IMFP (due to elastic scattering) ; usually

MED/cos θ > IMFP ; special case (due to DP, angle, etc)

2. Calculations of IMFPs in solids

- most 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 have made IMFP calculations **over 10 eV to 200 keV using relativistic full Penn algorithm (FPA)** from ELFs **for 41 elemental solids and 42 inorganic compounds.**

2. 1 Calculation of IMFPs from optical data - with relativistic full Penn algorithm

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

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

ELF(q, ω) by FPA : ω dependence ← experimental optical data (optical ELF)
: q dependence ← Lindhard model dielectric function (RPA)

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

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

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

Conditions for IMFP calculations: for making database

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 **optical ELFs** for materials**: 0.1 eV - 1MeV**

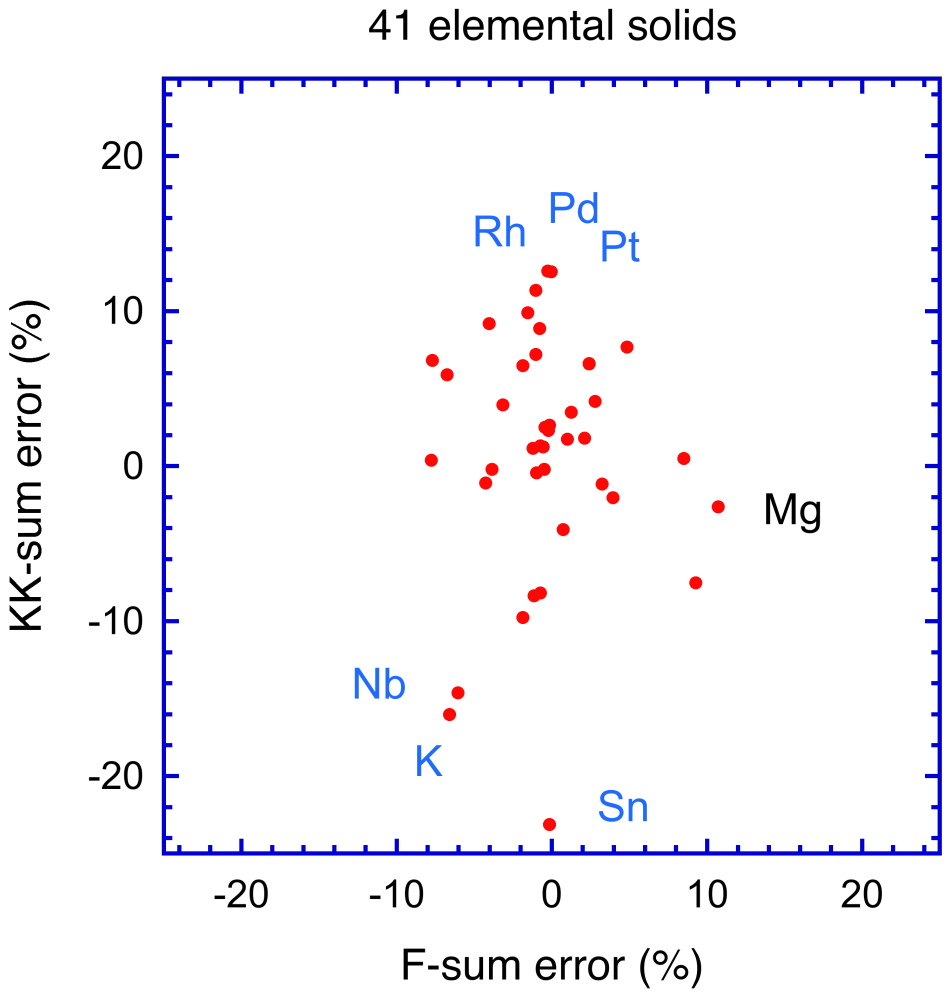
- 41 elemental solids

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.

- 42 in organic compounds

AgBr, AgCl, AgI, AlAs, AlN, AlSb, BN, BN(hex), CdS, CdSe, CdTe, GaAs, GaN, GaP, GaSb, GaSe, InAs, InP, InSb, PbS, PbSe, PbTe, SiC, SnTe, ZnS,, ZnSe, ZnTe, Al_2O_3, KBr, KCl, MgF_2, MgO, NaCl, $NbC_{0.712}$, $NbC_{0.844}$, $NbC_{0.93}$, SiO_2, $TiC_{0.7}$, $TiC_{0.95}$, $VC_{0.76}$, $VC_{0.86}$, $Y_3Al_5O_{12}$

Evaluation of ELFs (q =0) : elemental solids



: OCs from HOC I, II, III by Palik (<30 eV)
>100 eV atomic scattering factors
(Henke et al. and EPDL97 by) Cullen et al.)

- **F-sum : evaluate the ELF at high energy region**
- **KK-sum :evaluate the ELFs under 100 eV**

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

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

10

ELFs(q=0) : inorganic compounds

・Experimental ELF (optical constants) are lacking over 10 eV.

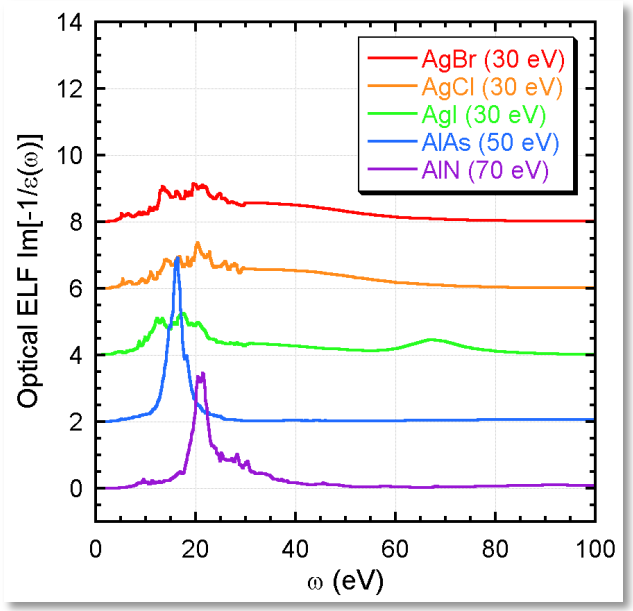
- Optical constants and ELFs for 30 compound semiconductors were calculated with **FEFF8.2 and WIEN2K in 0.1 eV – 1 MeV**.

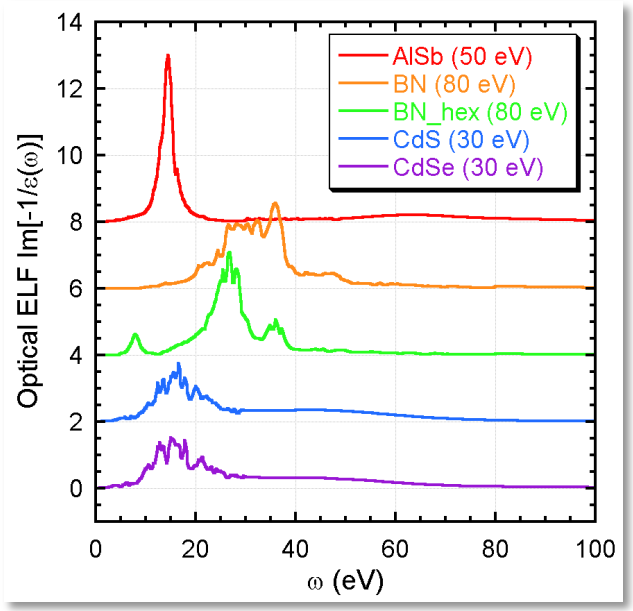
FEFF: Automated program to calculate the X-ray absorption spectra based on an ab initio all-electron, real space relativistic Green's function formalism
→ Available for inner-shell electron excitation

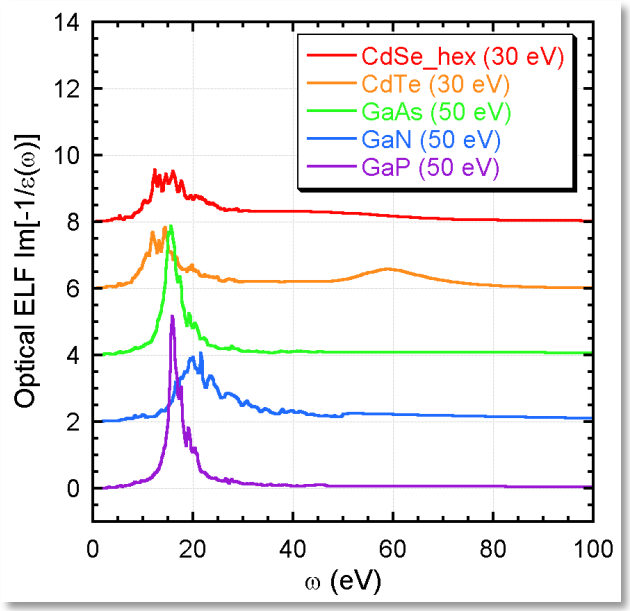
WIEN2K: Program package to perform the electron structure calculation based on density functional theory using full potential and linearized augmented plane wave method
→Available for valence electron excitation

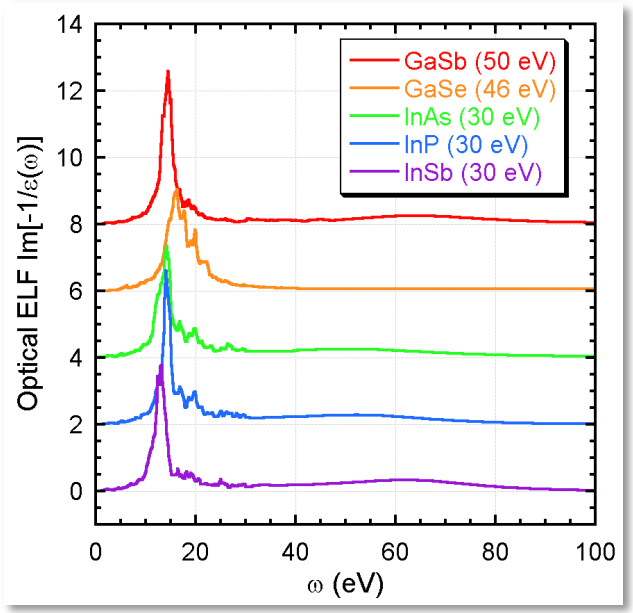
- Space group and cell parameters : ex. AgBr , F m -3 m, a = 5.775

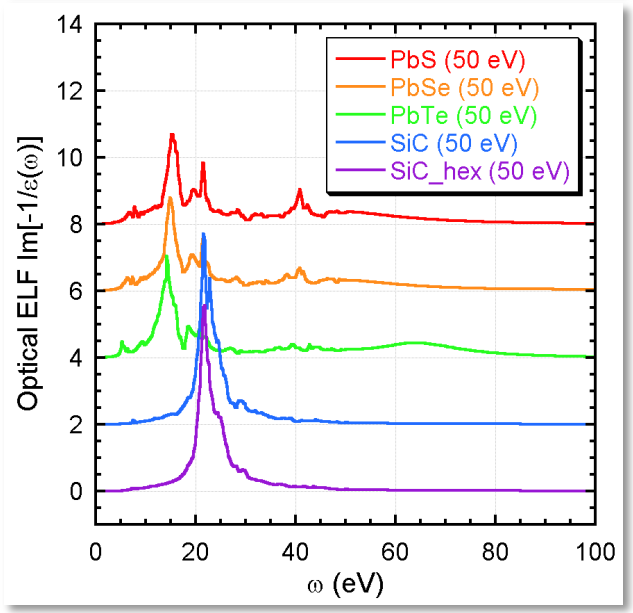
Calculated results of ELFs for 30 compounds: 0 -100 eV

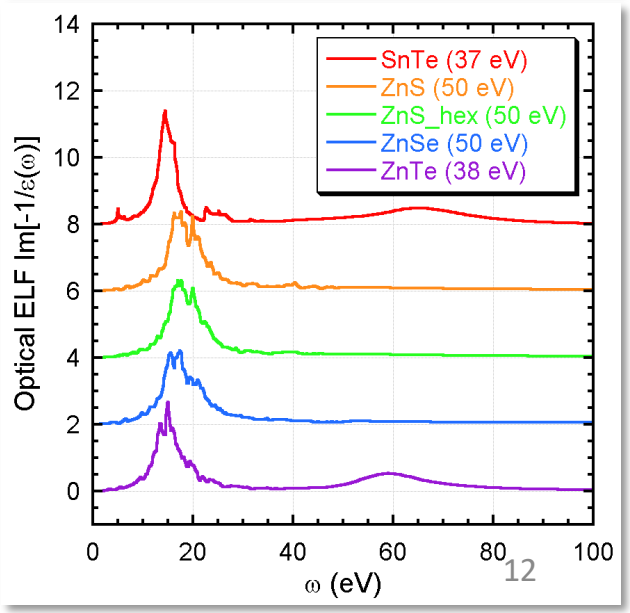




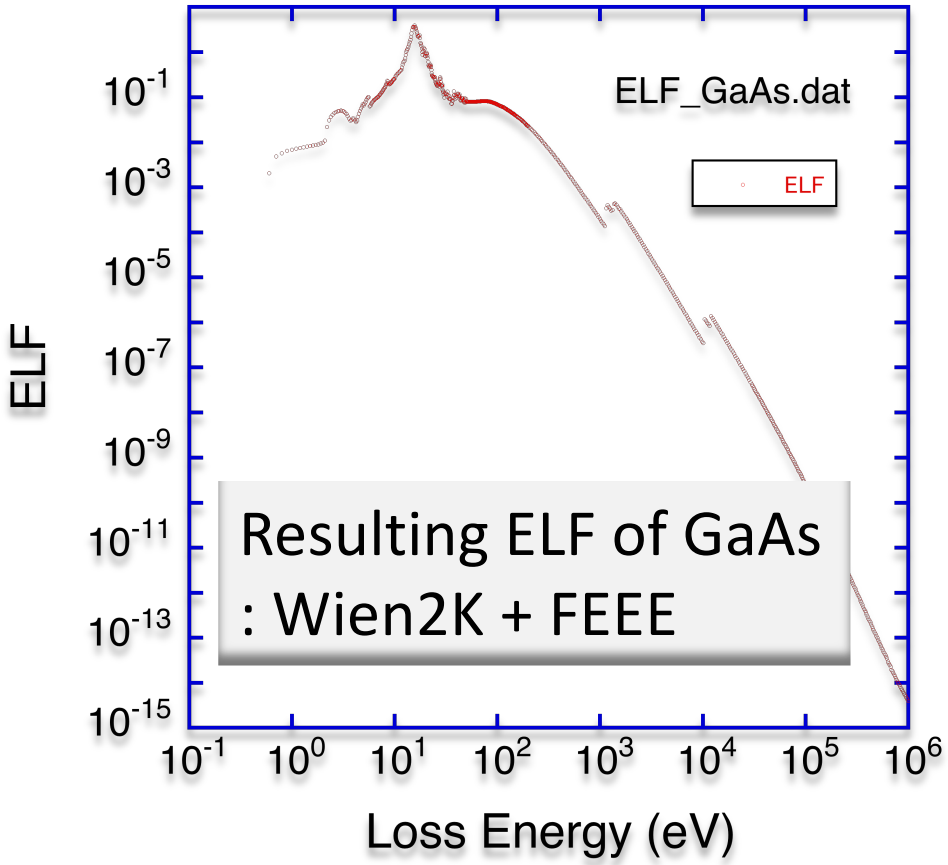




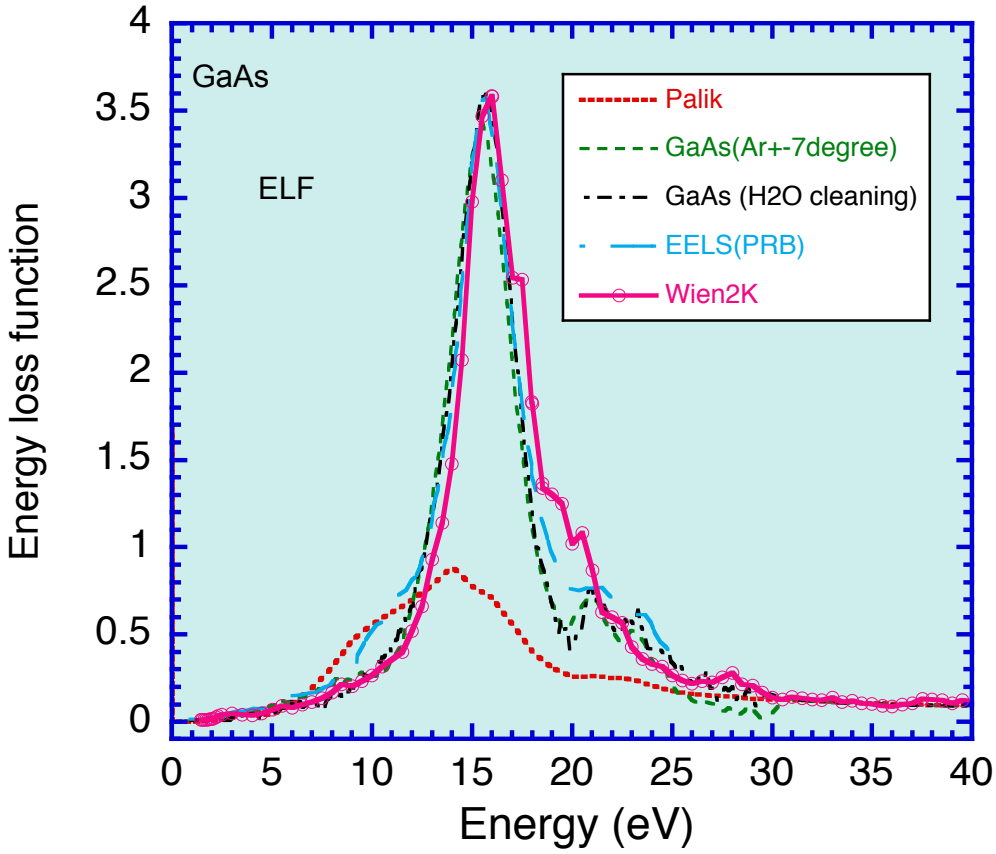




Evaluation: ELF for GaAs

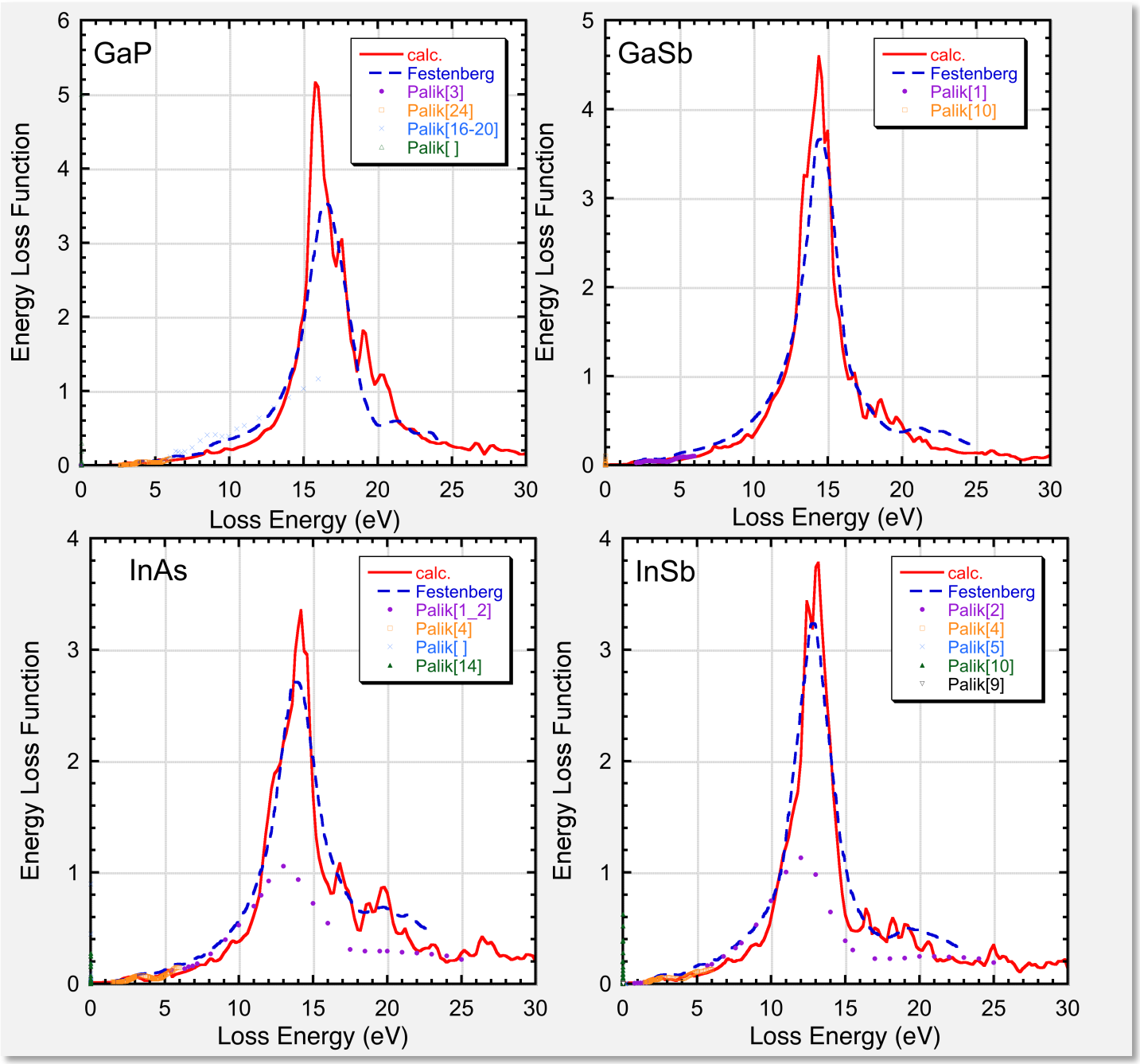


Comparison : ELFs from REELS +TEM



:Theoretical calculation (DFT: Wien2K) is in excellent agreement with the ELFs from AR-EELS (Jin – Yoshikawa et al) and TEM

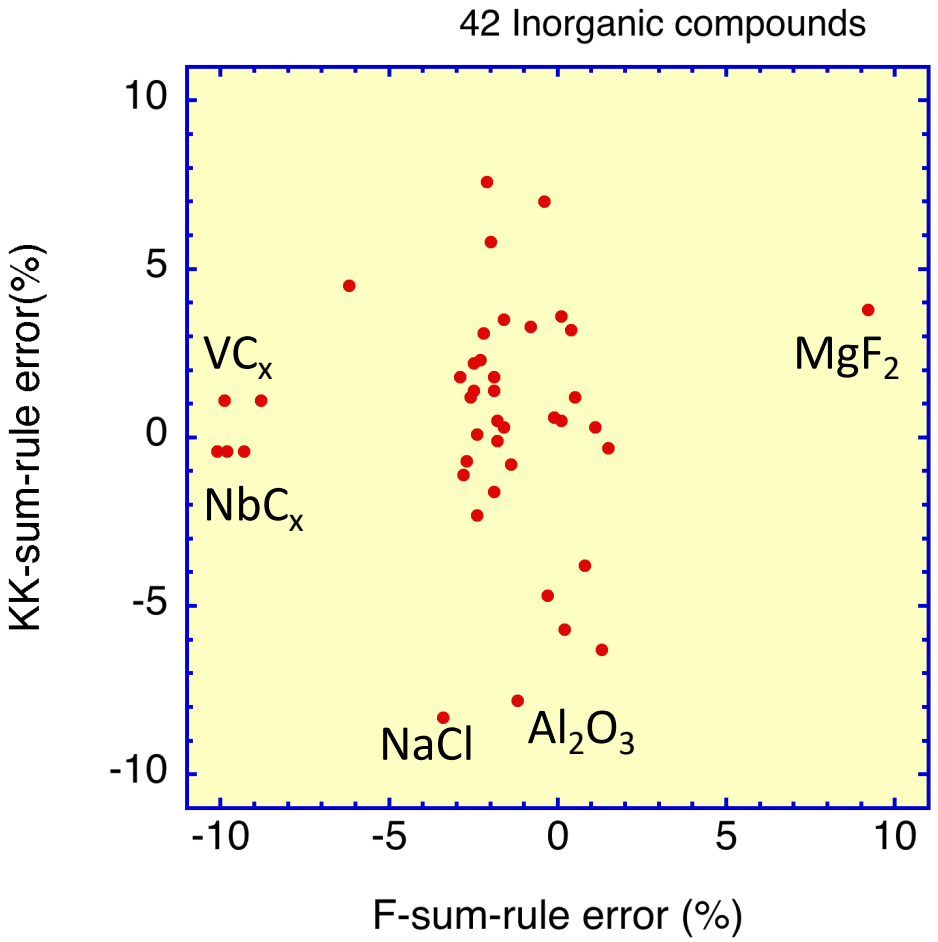
Comparisons of ELFs with TEM-EELS data

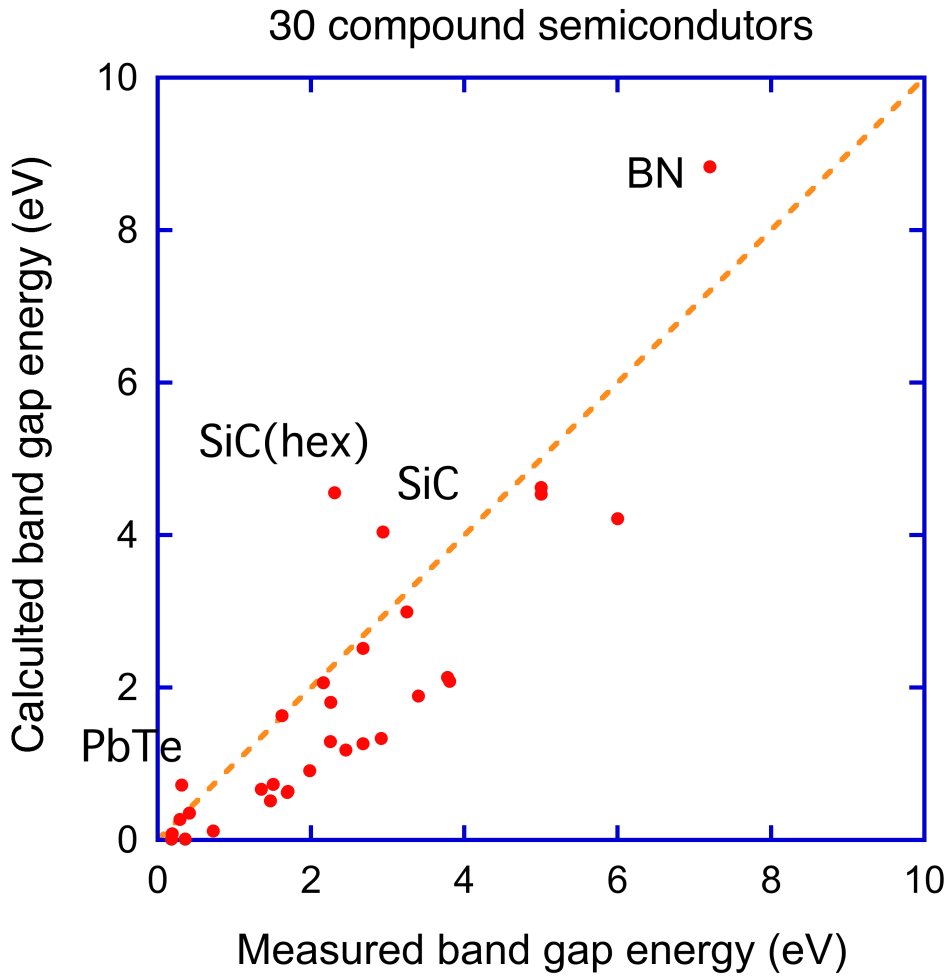


: good agreement
Wien2k – TEM (by Festenberg)

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

Evaluation of ELFs : 42 inorganic compounds

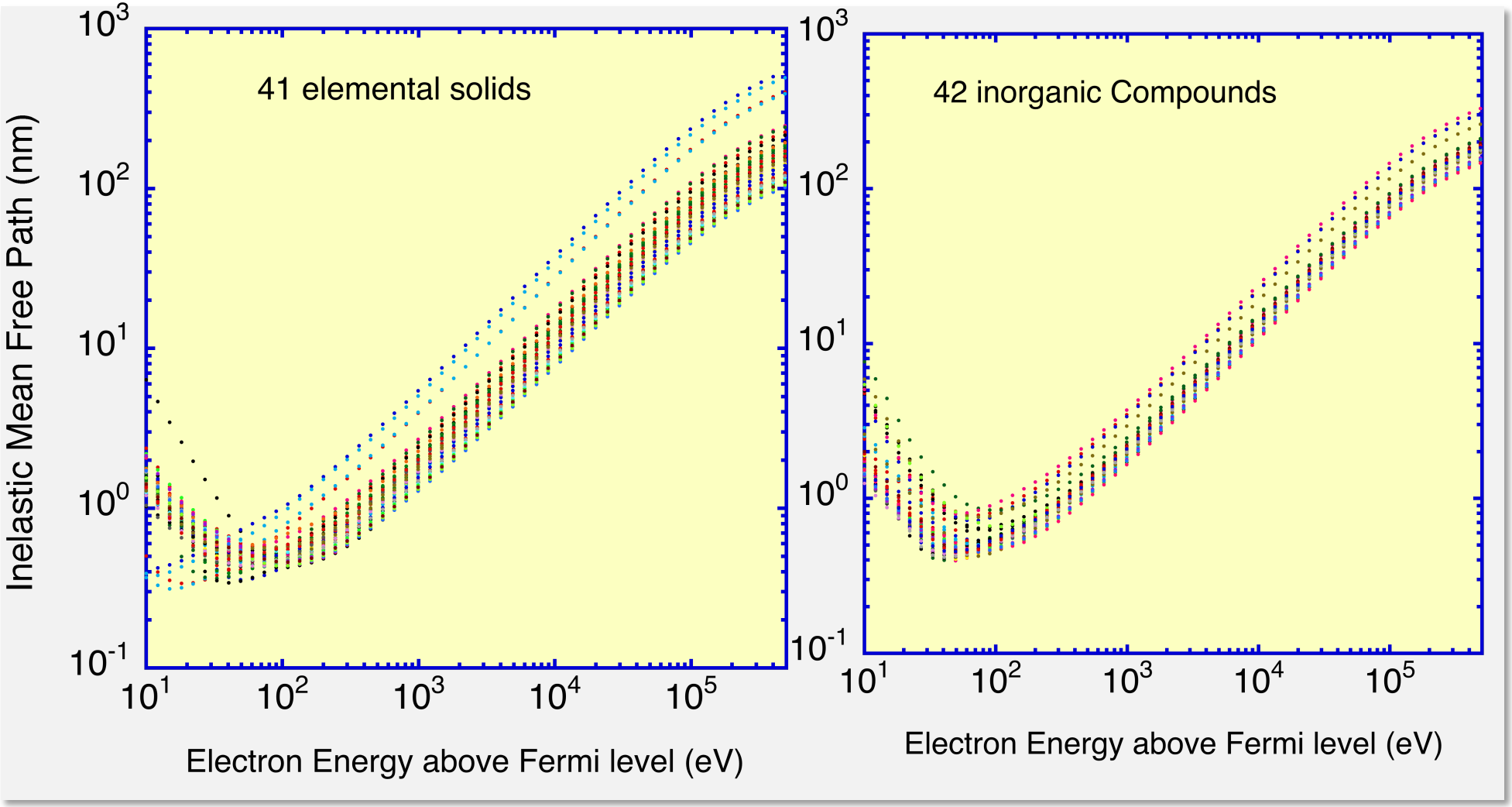




- For 32 of our 42 compounds, the f-sum-rule and KK-sum rule errors are both less than 5 %.

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

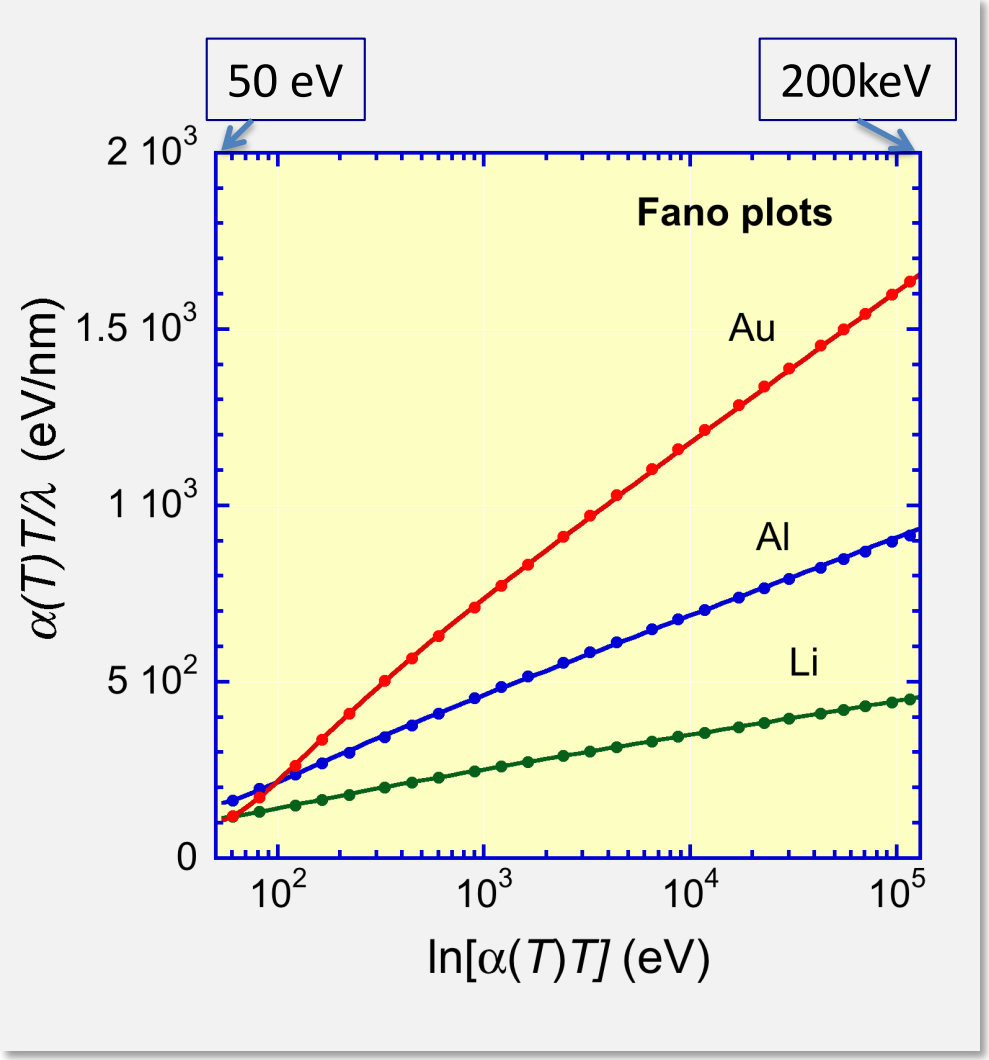
Calculated results of IMFPs : 10 eV – 200keV



Factor: 17.3 at 10 eV
2.4 at 100 eV
4.2 at 1 keV

Factor: 6.1 at 10 eV
2.0 at 100 eV
2.2 at 1 keV

Fano plots and Curve fits for elemental solids



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

Solid lines: Fit with Rel. mod. Bethe equation

Energy range: 50 eV – 200 keV

β, γ, C, D : fitting parameters

RMS differences (%)

Li : 0.31

Al : 0.82

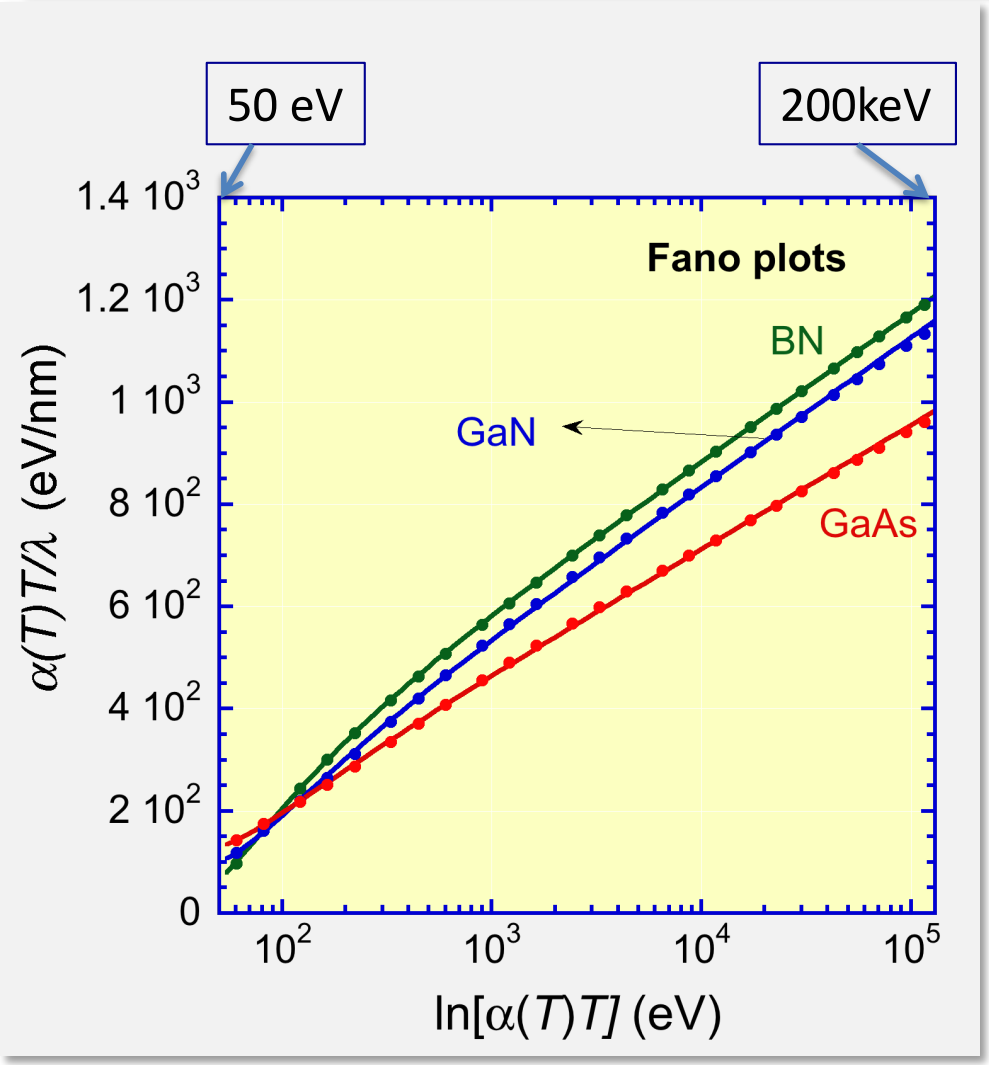
Au : 0.47

Average of RMS (%) for 41 elemental solids

0.68% (0.4 – 1.4 %)

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

Fano plots and Curve fits for inorganic compounds



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 : 0.50

GaN : 0.92

GaAs : 0.93

Average of RMS (%) for 42 compounds

0.59 % (0.2 – 1.1 %)

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

Relativistic TPP-2M equation

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

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

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

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

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

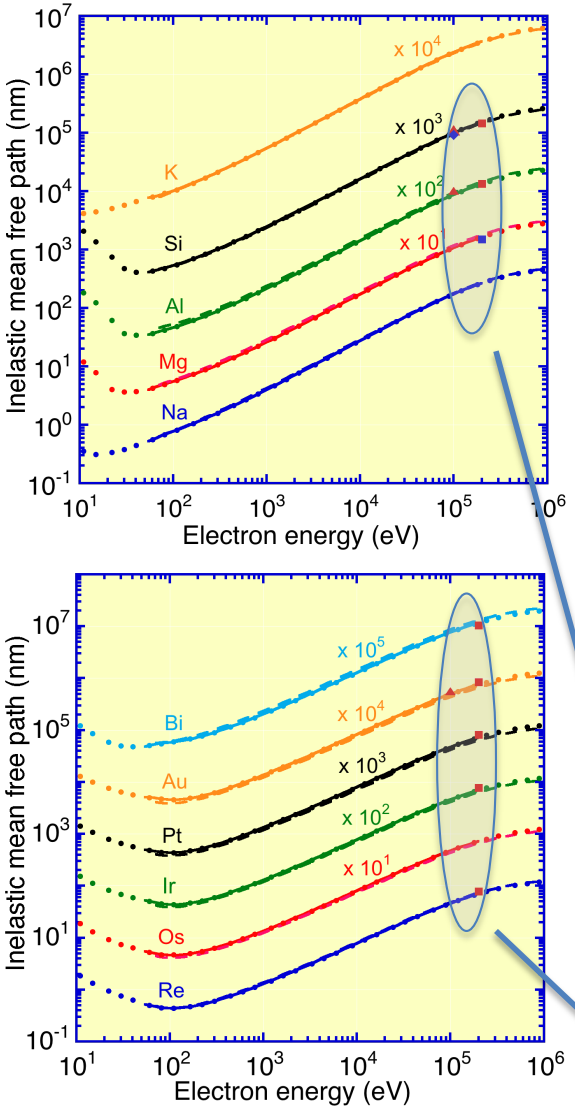
$$\alpha(T) = \frac{1 + T/\left(2m_e c^2\right)}{\left[1 + T/\left(m_e c^2\right)\right]^2}$$

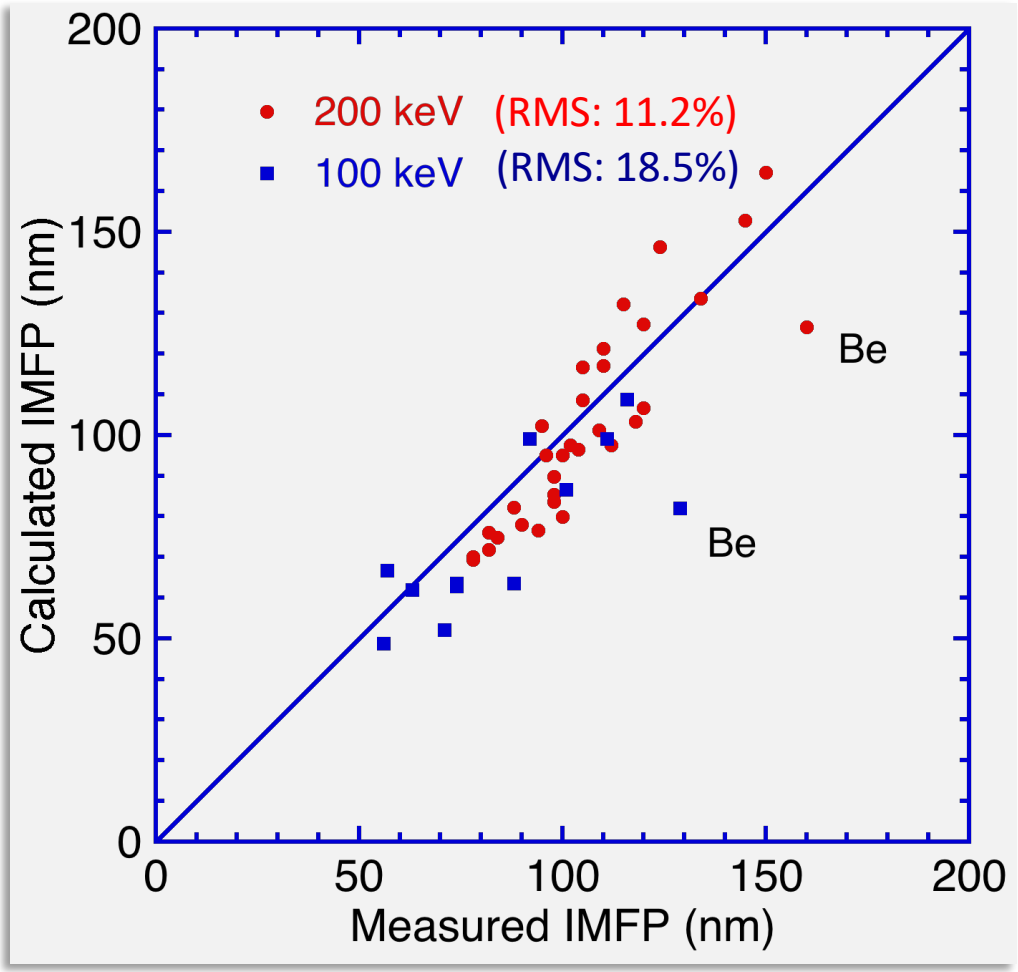
Energy range : 50 eV – 200 keV

Average of RMS (%) for 41 elemental solids ➔ 11.9 %
(8.9% ; except for diamond, graphite, Cs)

Average of RMS (%) for 42 inorganic compounds s
10.7 % (2.4 – 66 %)
8.9 % (except BN)

Comparison of IMFPs with experimental results

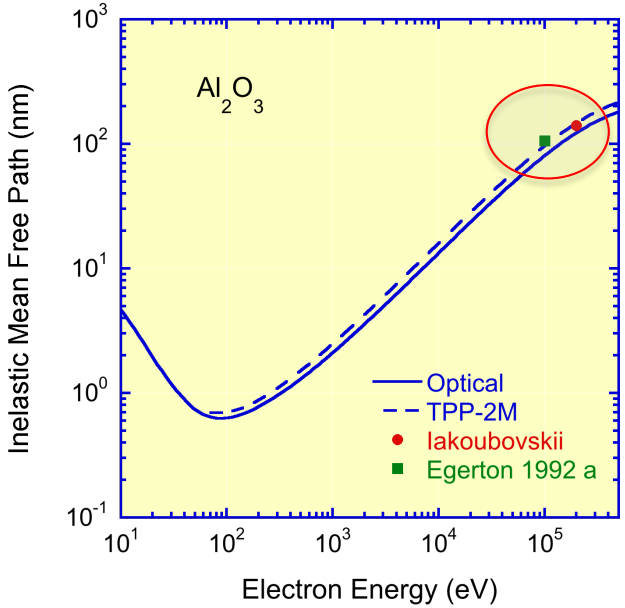


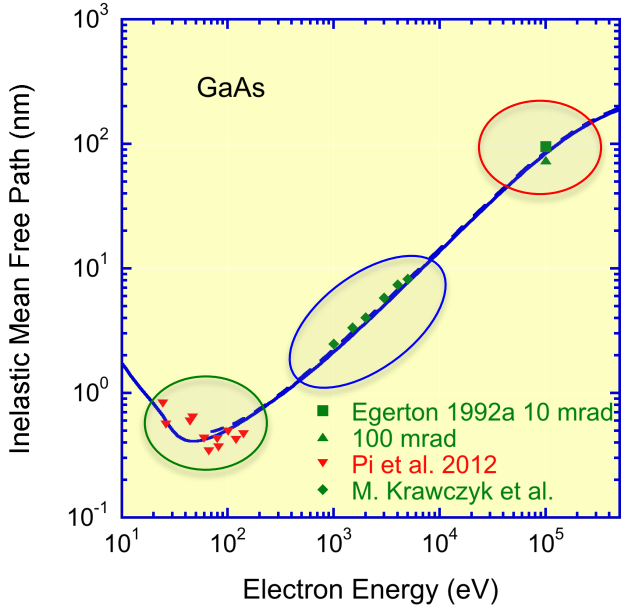


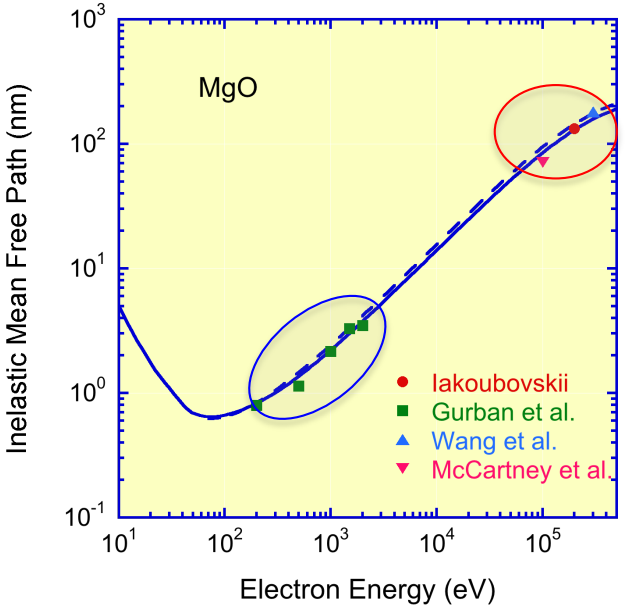
Solid marks: measured by TEM

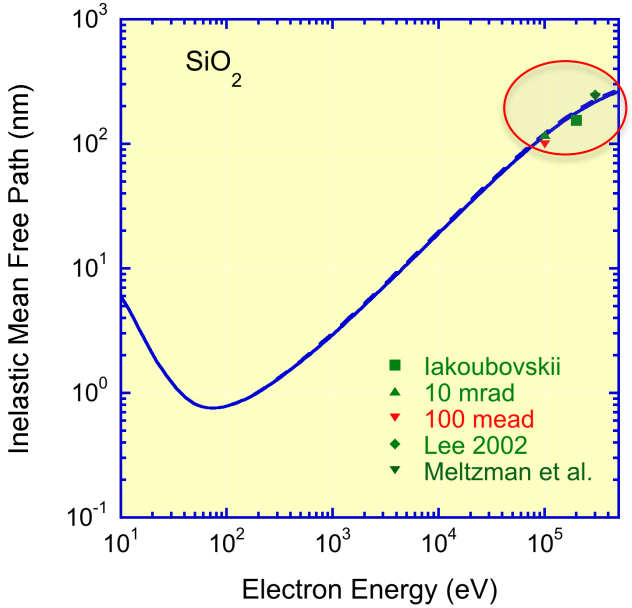
Experimental : TEM
100 keV: 11 elemental solids
200 keV: 32 elemental solids

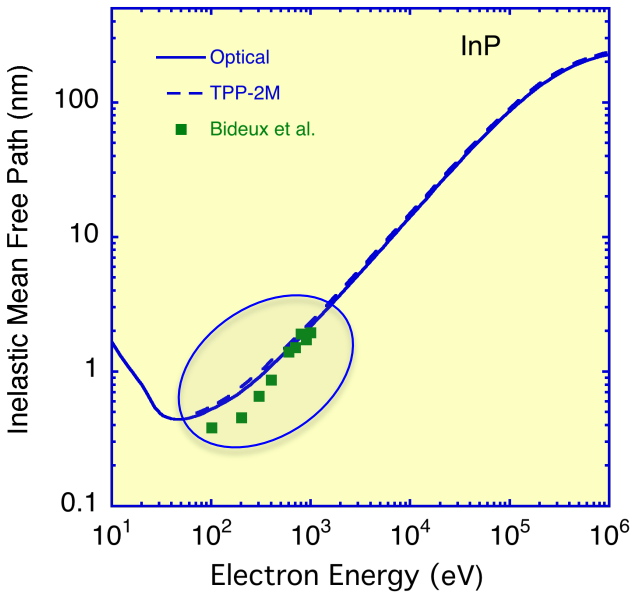
Comparison of IMFPs for compounds with experimental results











Solid line: optical IMFPs
Dotted line: rel. TPP-2M

TEM: Iakoubovski, McCartney
Egerton, Lee, Mellzman, Wang

EPES: Krawczyk, Gurban(SEC)
Bideux

SR-XPS: Pi,

3. Measurements of IMFPs in solids
- EPES experiments (10 eV – 5keV)

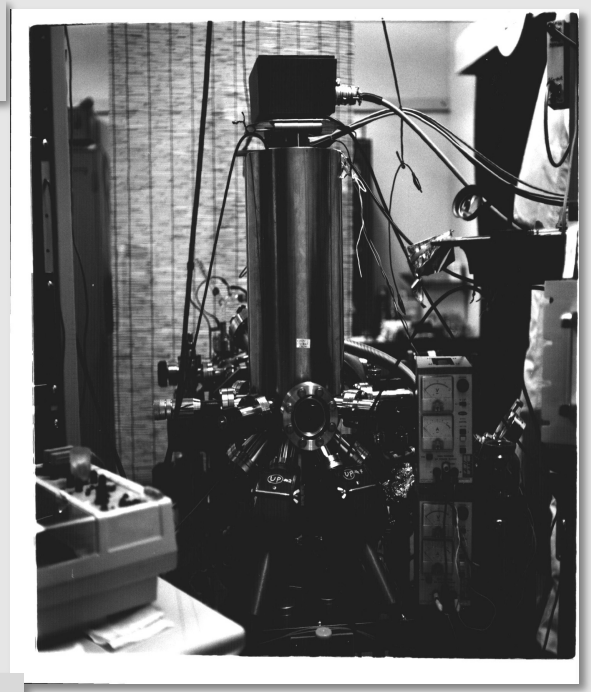
: to know the reliability of IMFPs calculated from ELFs with Penn algorithm (optical IMFP) and from TPP-2M.

- 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 (Ratios)**

-determine IMFPs for several elemental solids and compounds **from absolute EPIs over 10 eV – 5 keV**

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

Measurements of EPIs by absolute CMA



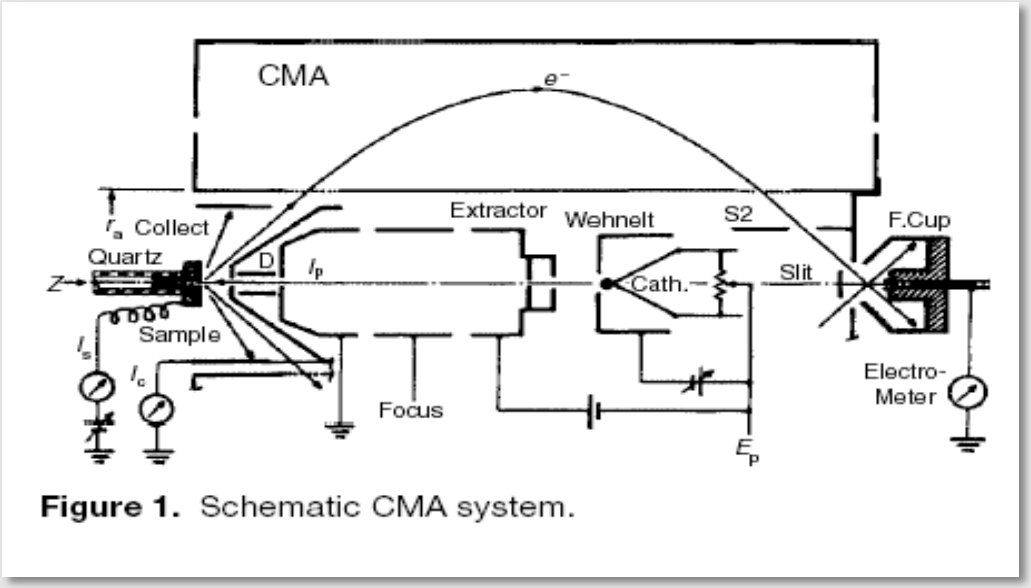


Figure 1. Schematic CMA system.

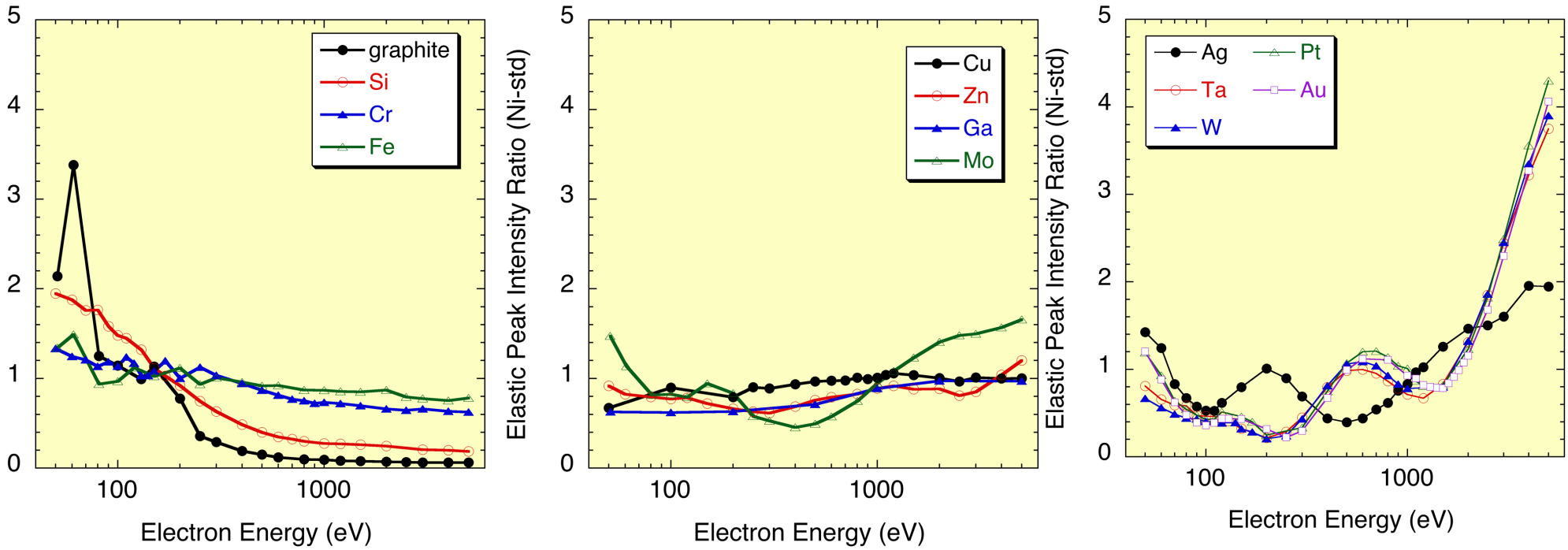
CMA ΔE/E = 0.25%

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

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



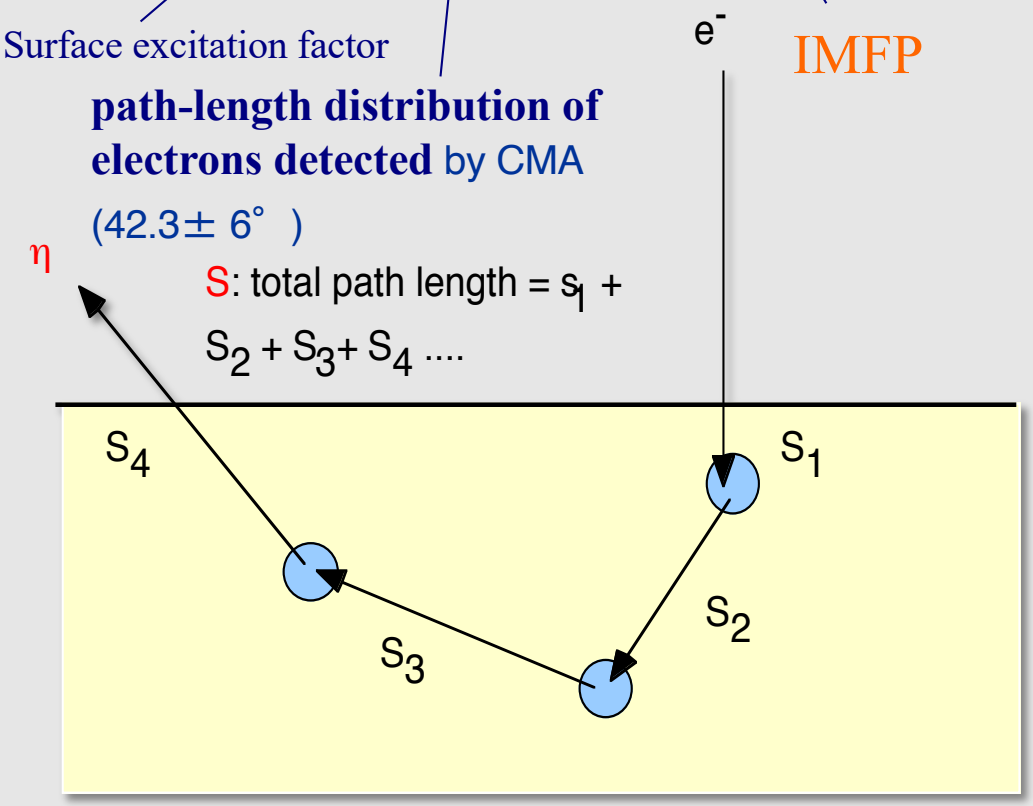
Calculation of EPI with MC method

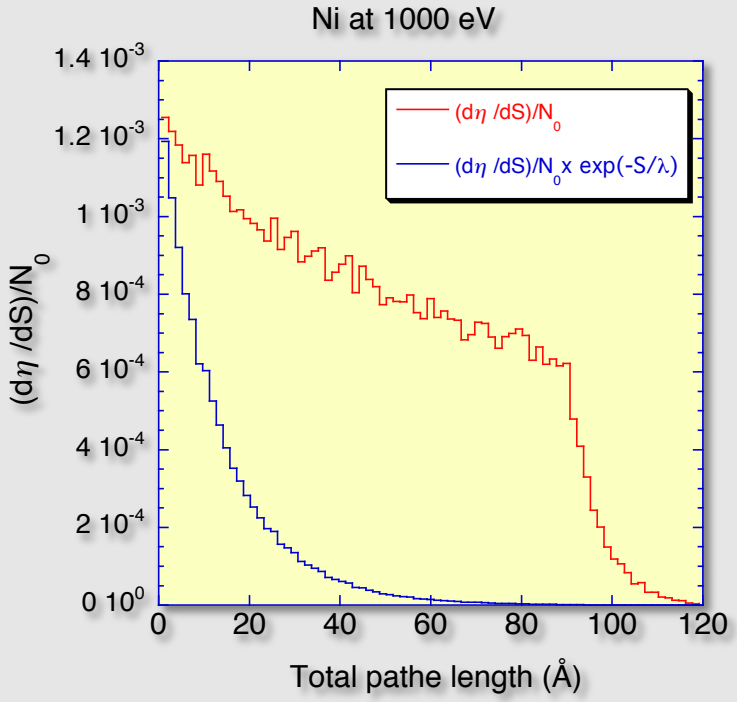
$$I = G_t \times f_s \times \int_0^{\infty} \left(\frac{d\eta}{dS}\right) / N_0 \exp\left(-\frac{S}{\lambda}\right) dS$$

Surface excitation factor

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

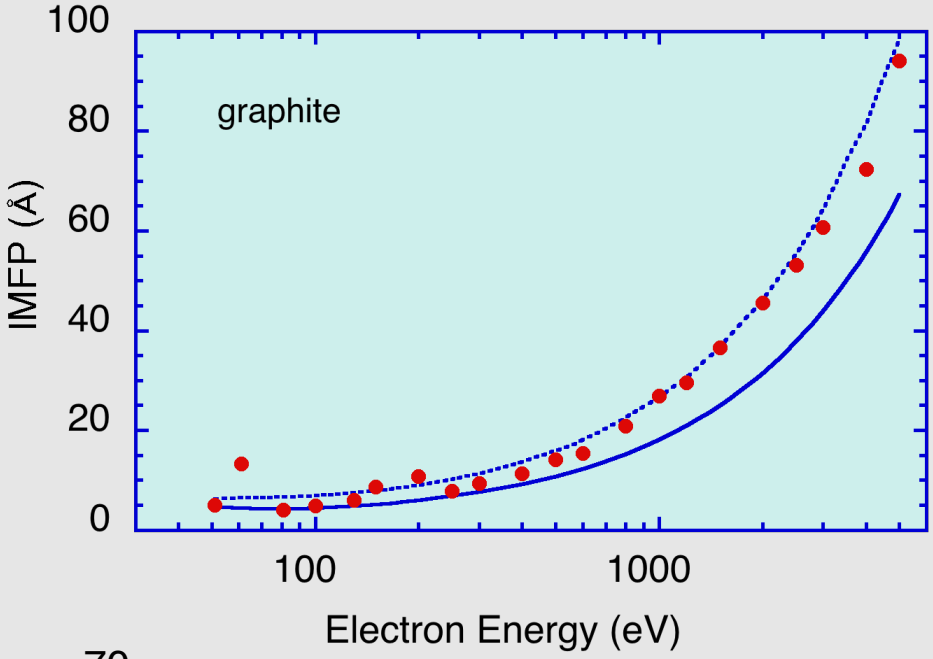
IMFP

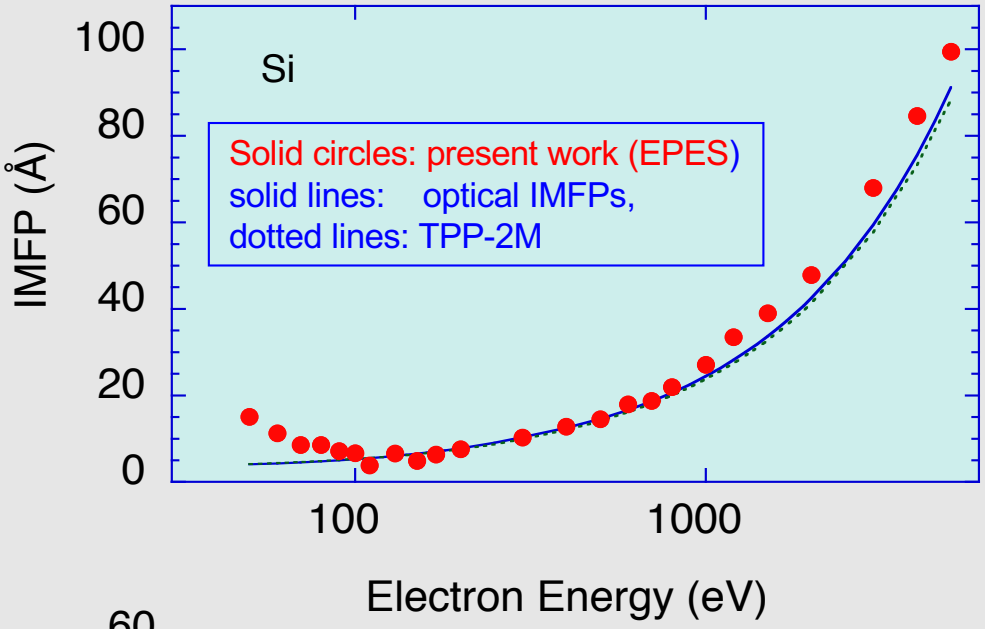


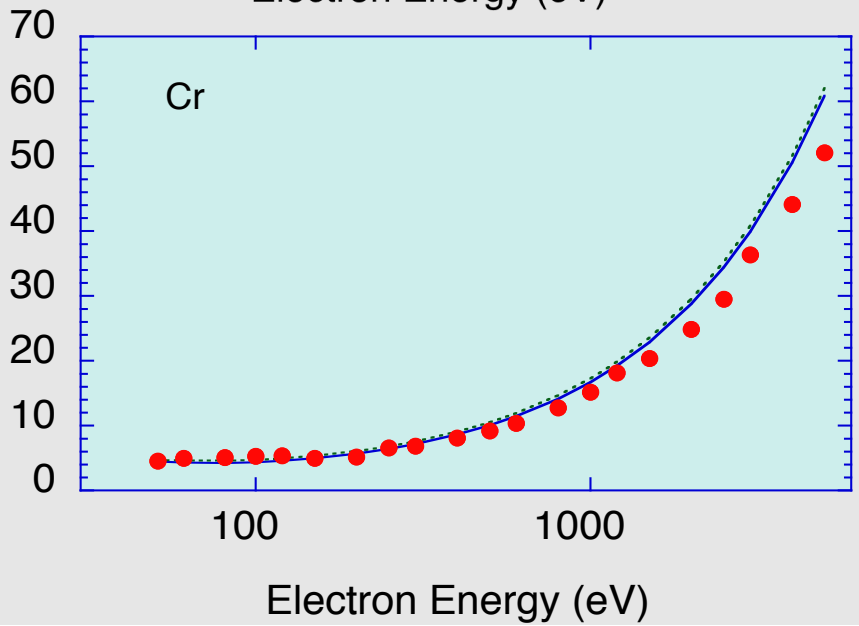


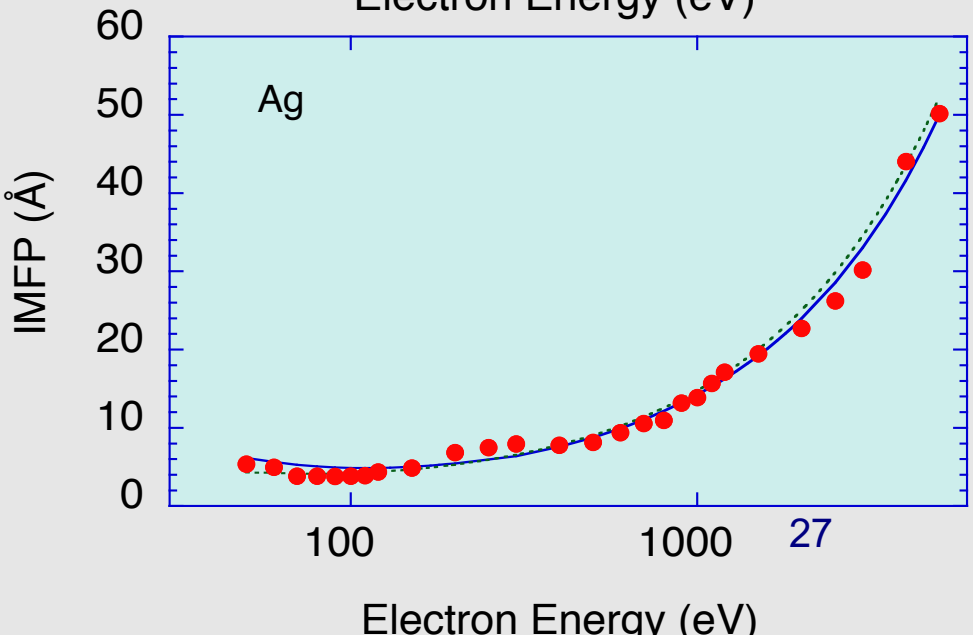
:Elastic scattering cross section
TFD or DHF potential

IMFPs determined from EPI ratios (Ni-ref)

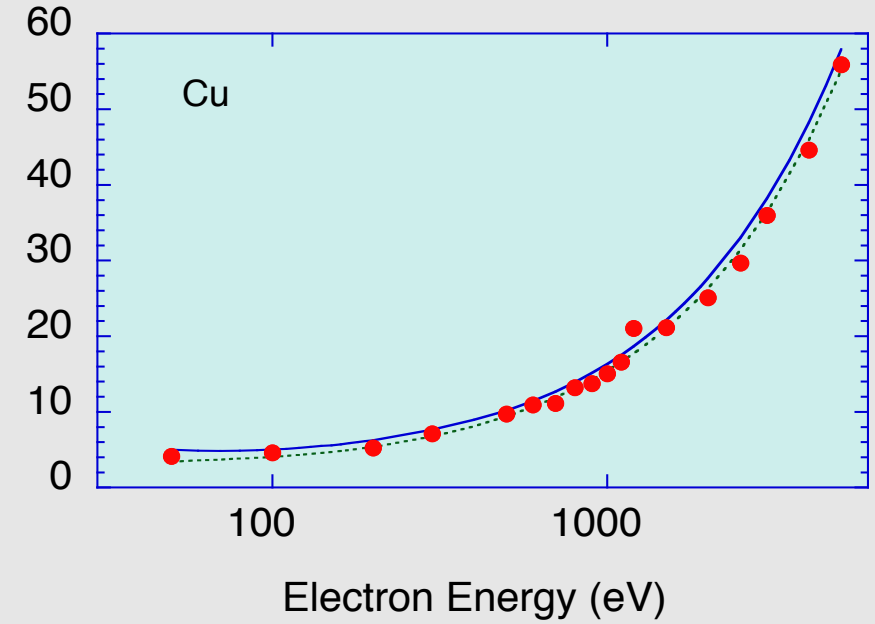


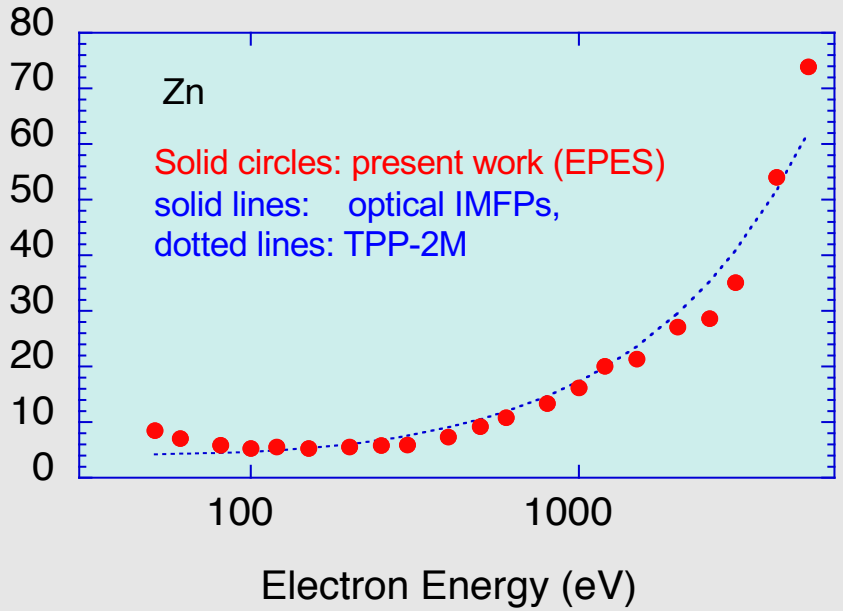


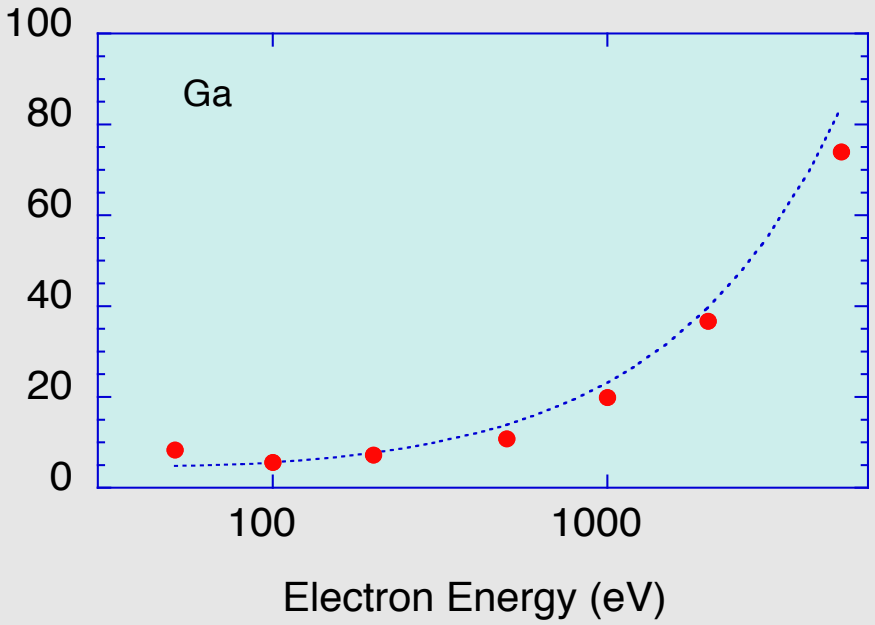


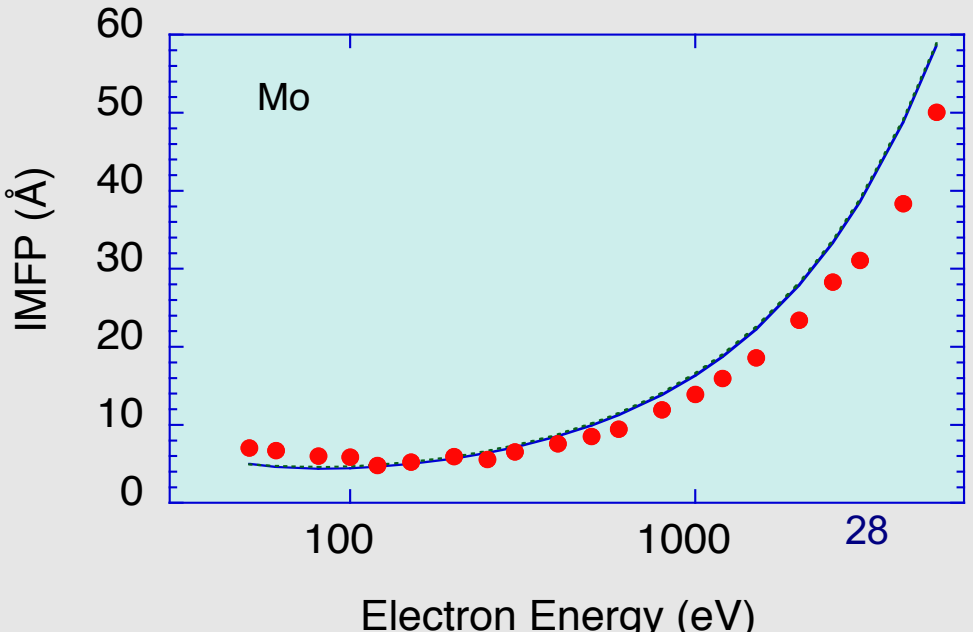


IMFPs determined from EPI ratios (Ni-ref)

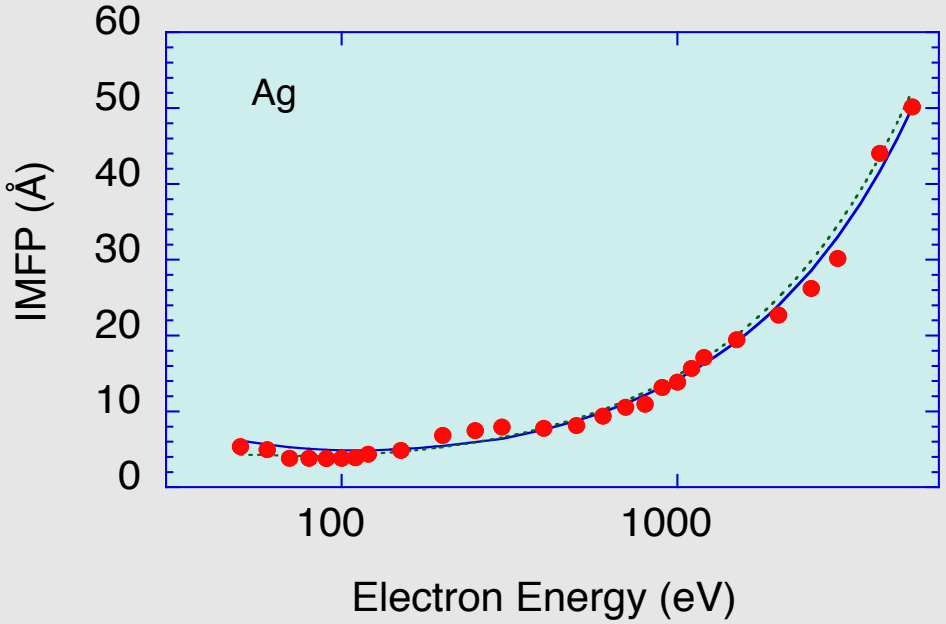


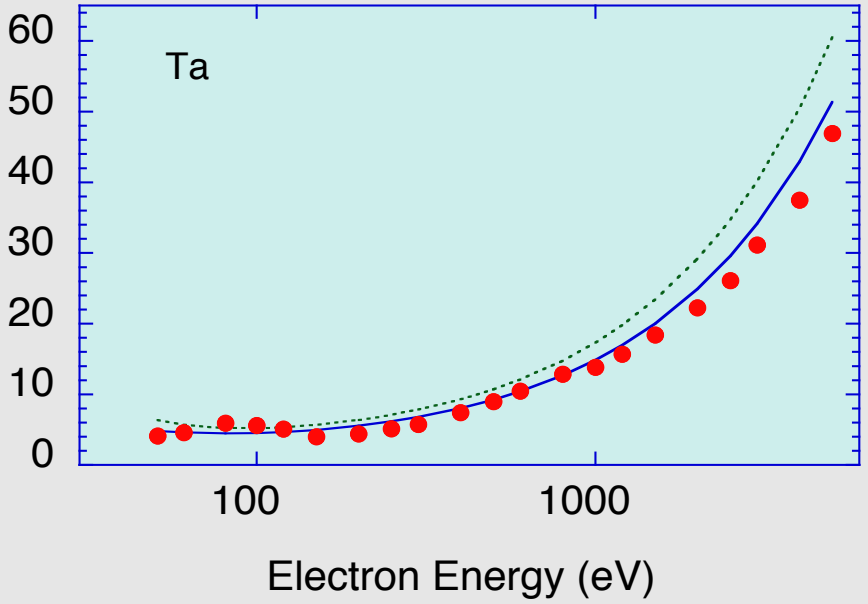


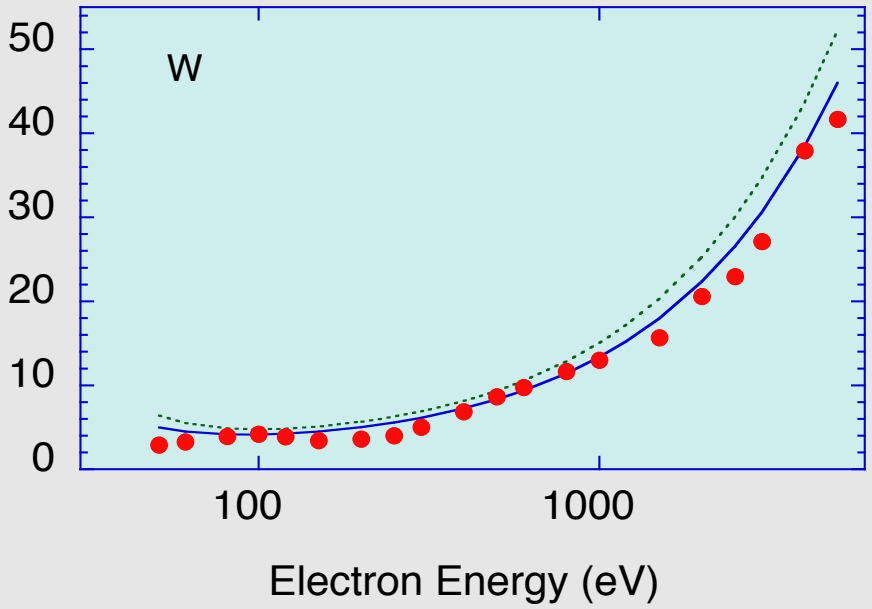


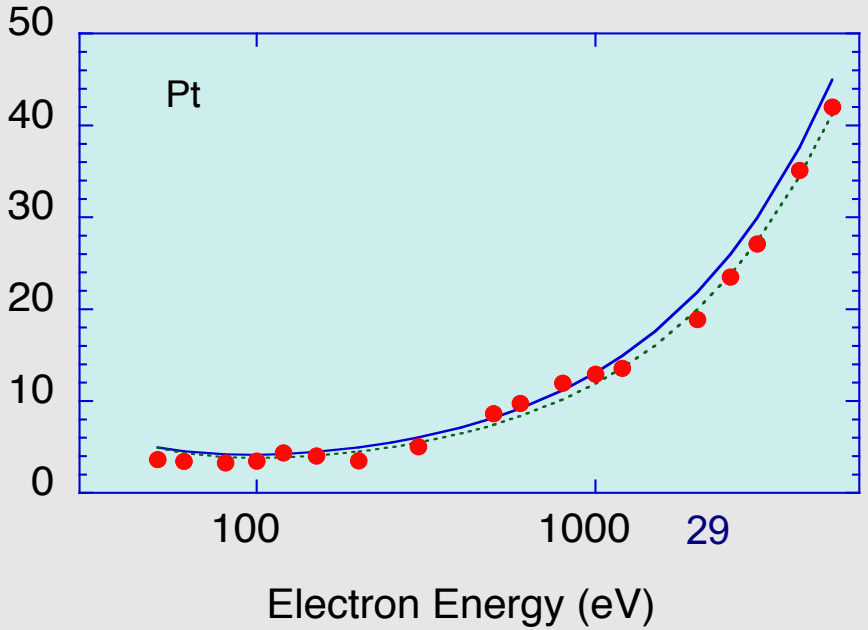


IMFPs determined from EPI ratios (Ni-ref)

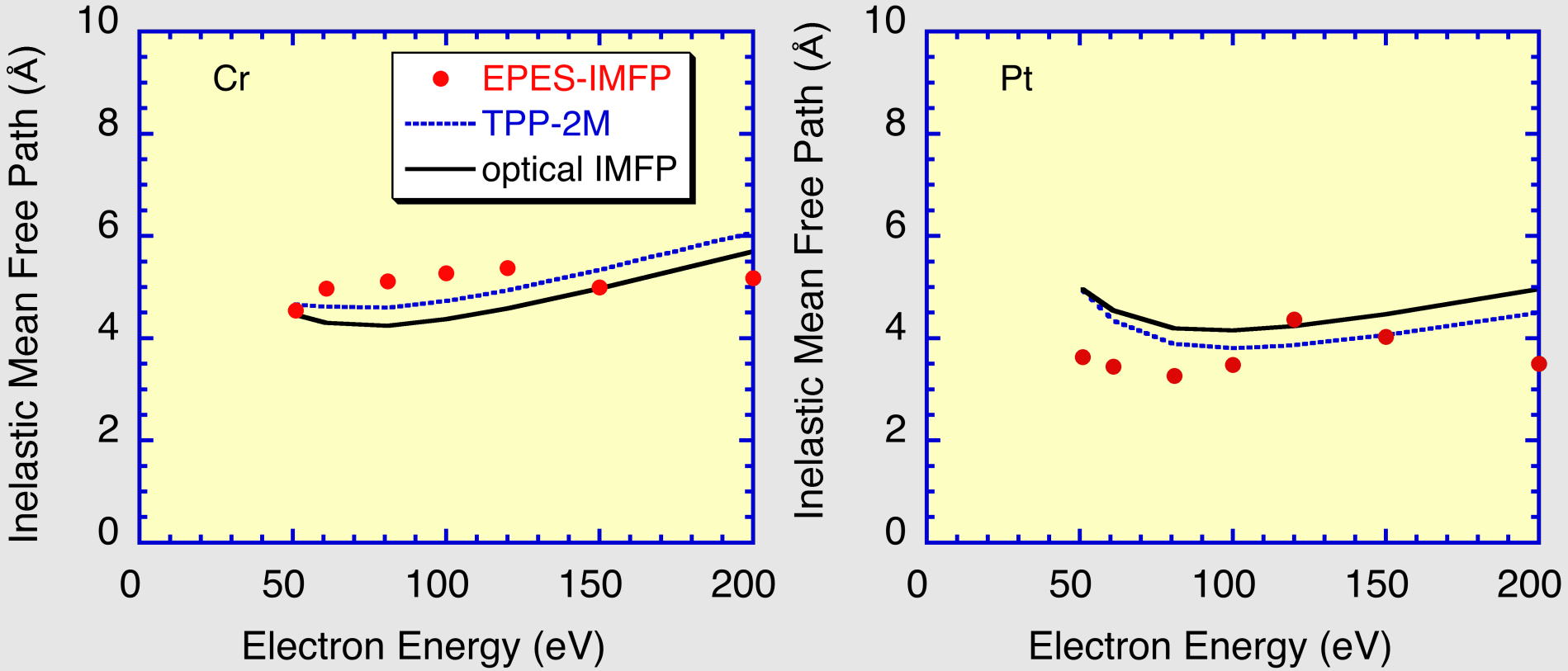






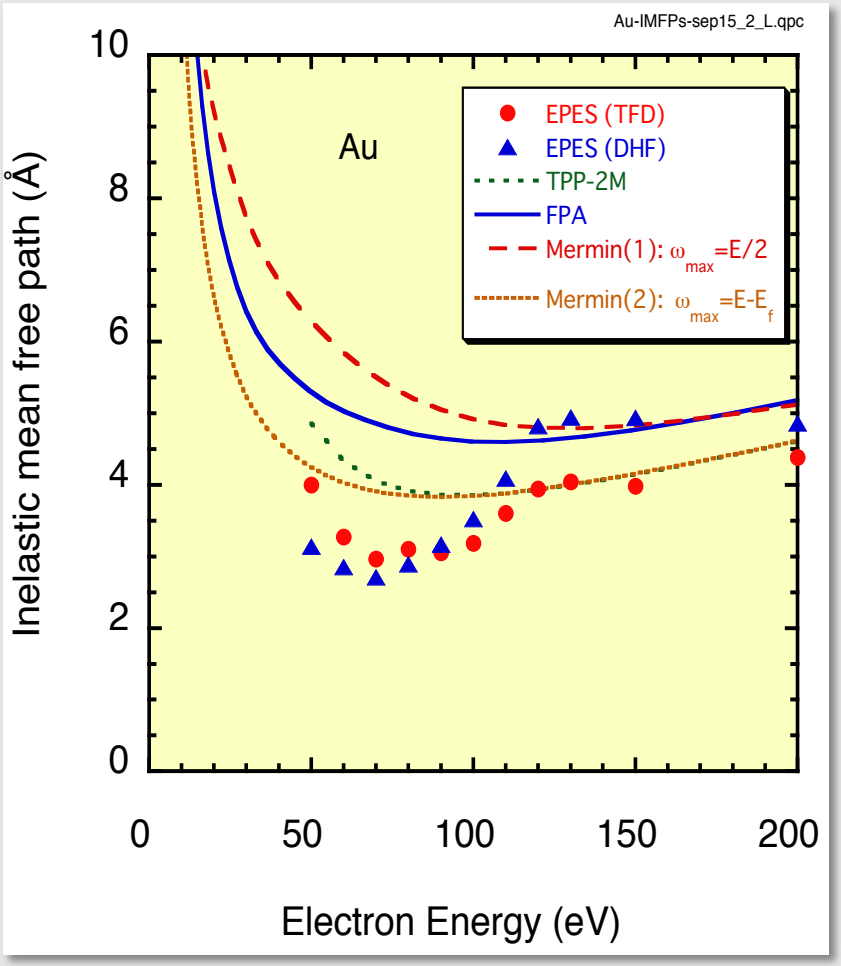


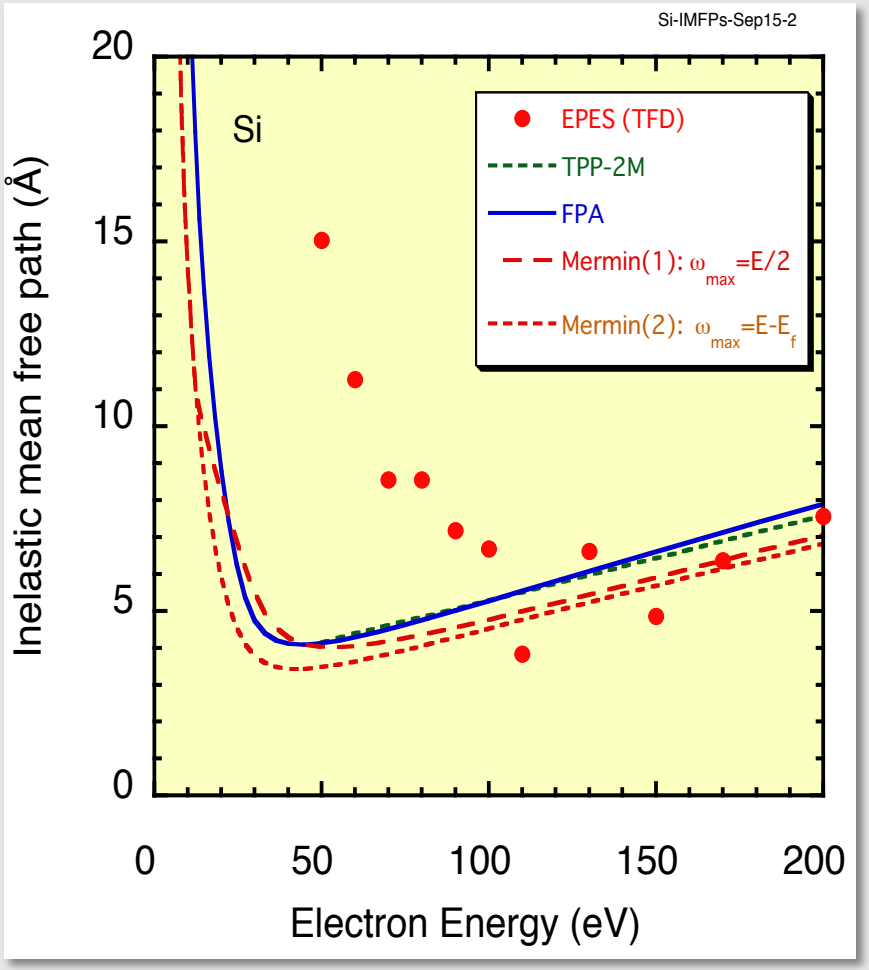
Comparison of IMFPs from EPES experiments at low energy region **(under 200 eV): Ni-ref**



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

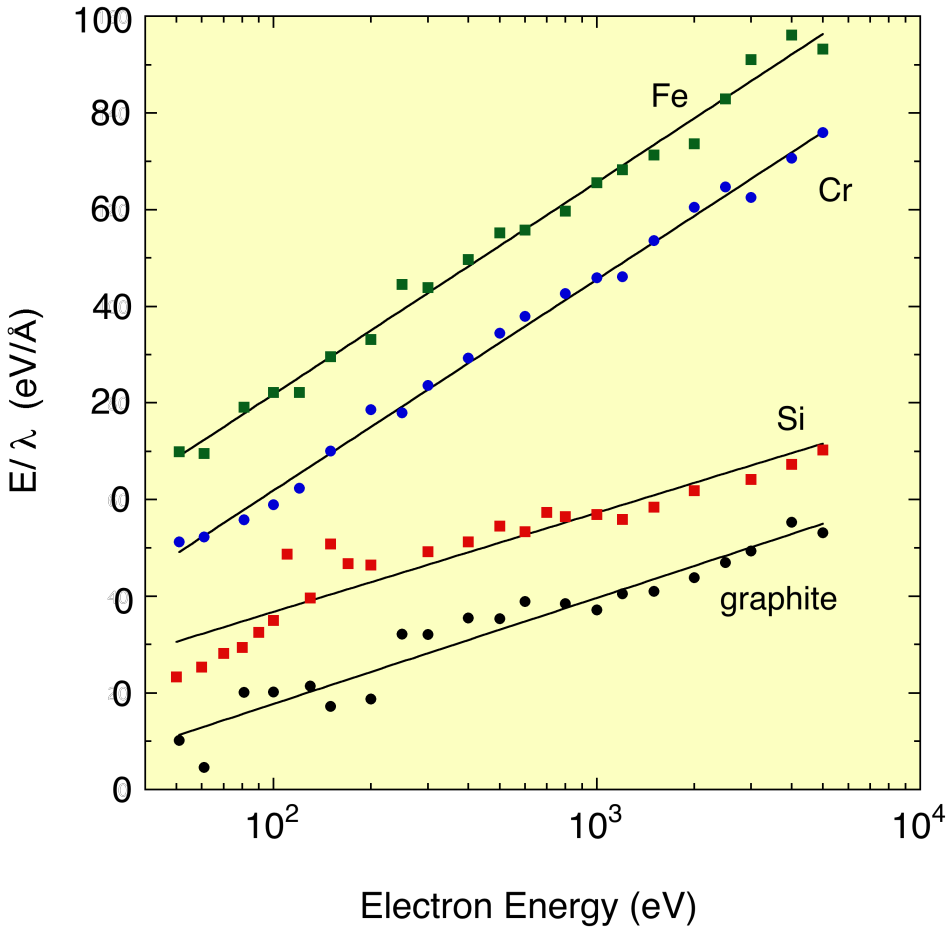
Comparison of IMFPs from EPES experiments at low energy region (under 200 eV): Ni-ref

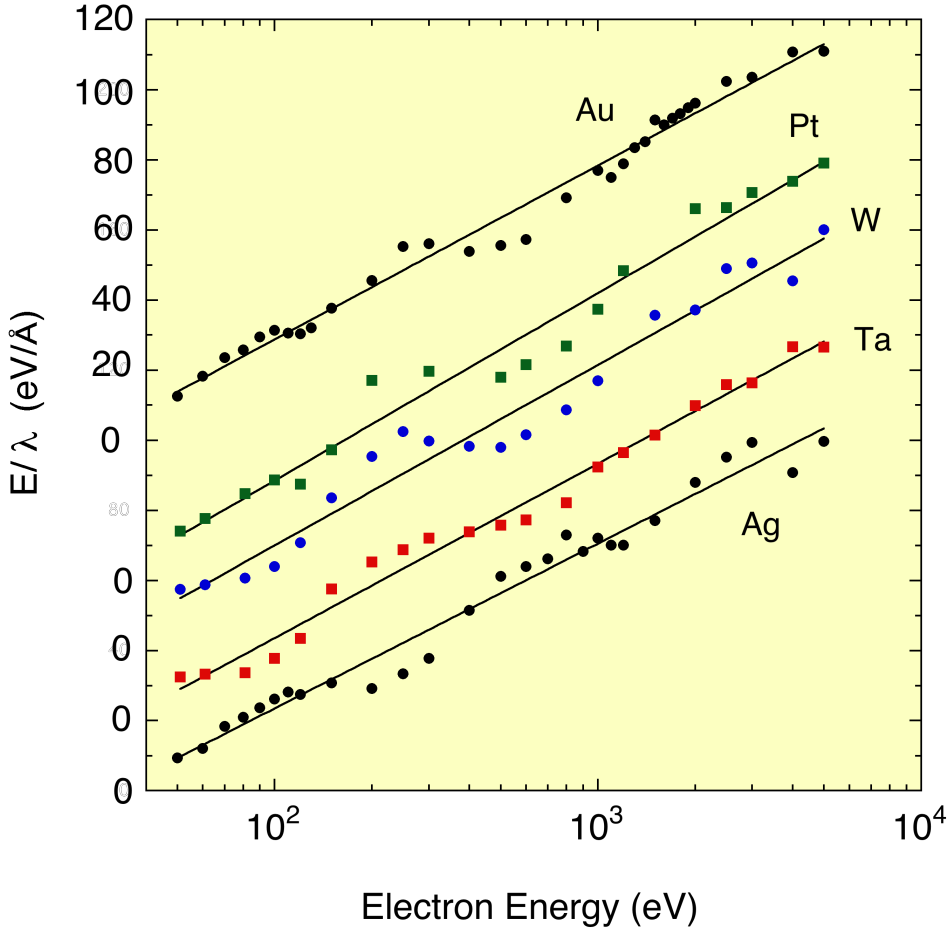




* surface excitation effect for EPES * IMFP values of Ni STD at low energy
* electron exchange effect , correlation effect

Analysis of IMFPs with Fano Plot





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

Simple Bethe equation

32

Comparison of calculated and measured **absolute** EPIs over 10 eV – 5 keV

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

Gt (transmission function) and f_s
- correct values are required

- to be determined without reference material

G_t : Measured transmission efficiency of CMA

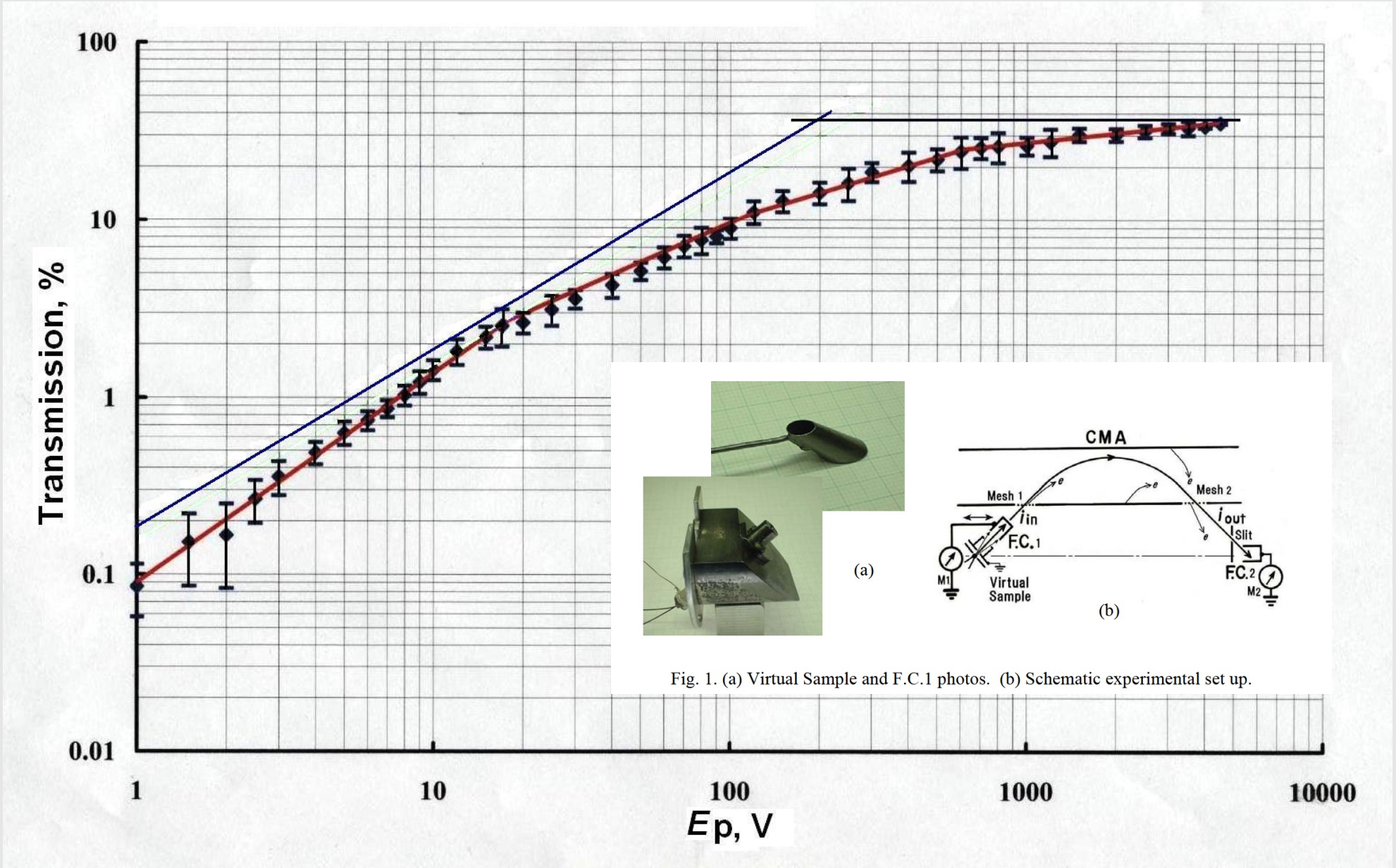
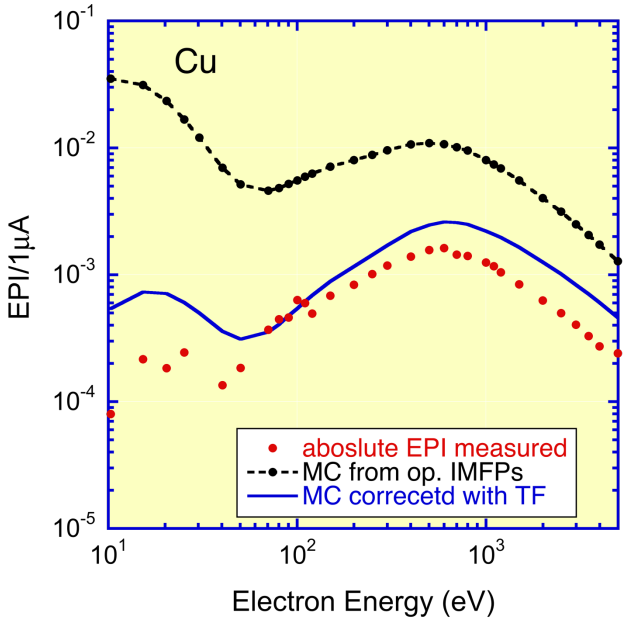
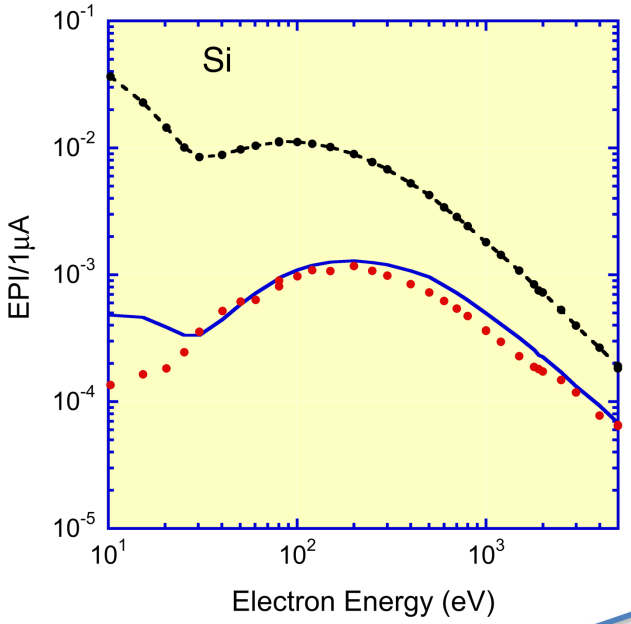
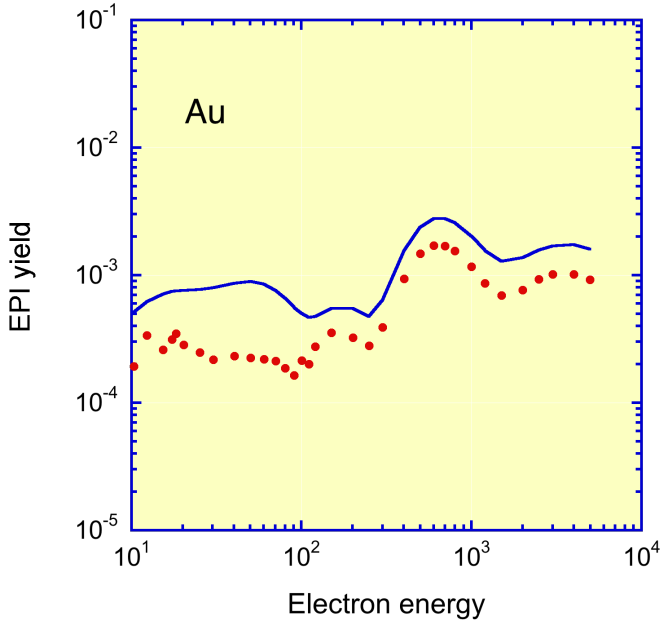


Fig. 1. (a) Virtual Sample and F.C.1 photos. (b) Schematic experimental set up.

Absolute EPI without SEE







? : estimations of f_s and λ

Red solid circles: measured EPI

Black line : I (Gt =1, fs =1)

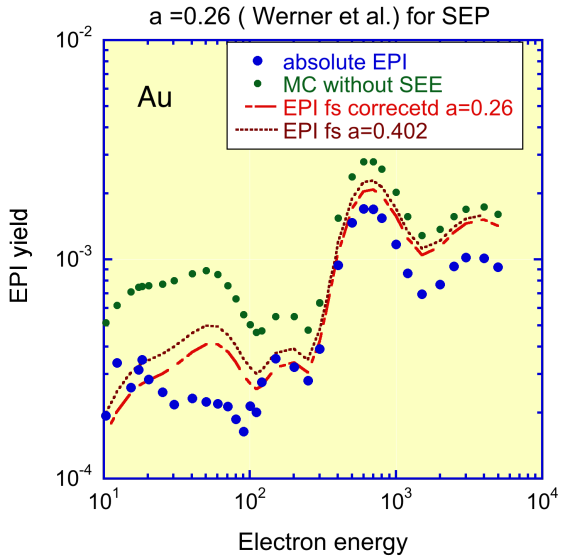
Blue solid line:

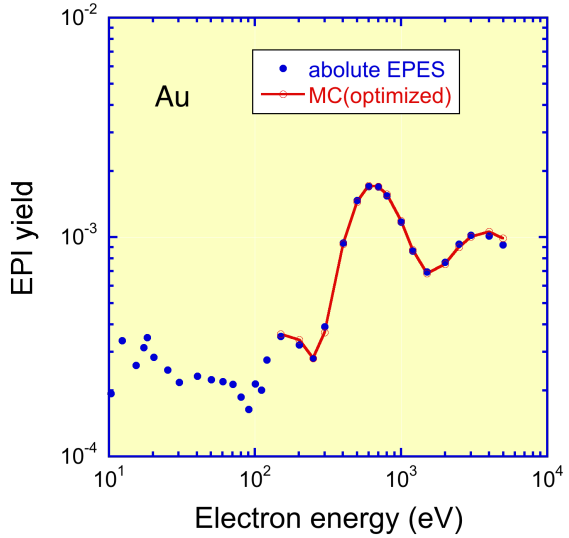
$$I = G_t \times (f_s = 1) \times \int_0^{\infty} \left(\frac{d\eta}{dS} \right) / N_0 \exp\left(-\frac{S}{\lambda} \right) dS$$

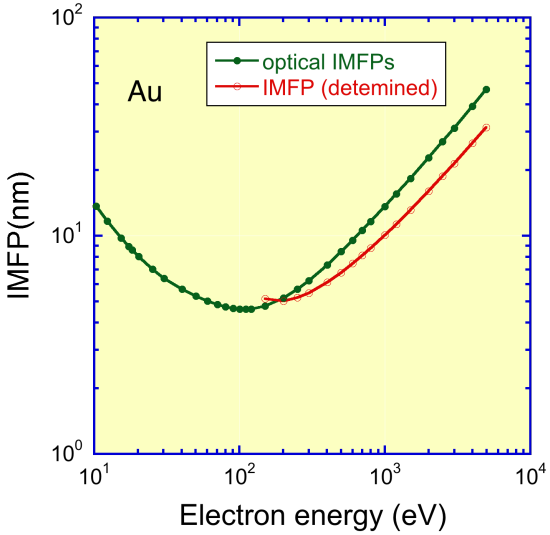
Gt: measured

Optical IMFP by FPA

Absolute EPI (3-paremeters) ≥150 eV







Optimize (fs and λ with 3 parameters; *a*, β, γ)

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

$a = 0.29 \quad (0.26;\ \text{Werner})$

$\beta = 0.413 \quad (0.2071;\ \text{optical IMFP})$

$\gamma = 0.0146 \quad (0.0577)$

$RMS(\%) = 3.4$

Oswald-Werner equation

$$f_s = \exp(-P_s), \quad Ps = \frac{1}{a\sqrt{E}\cos(\alpha_{in})+1} + \frac{1}{a\sqrt{E}\cos(\alpha_{out})+1}$$

Parameter described by Bethe equation

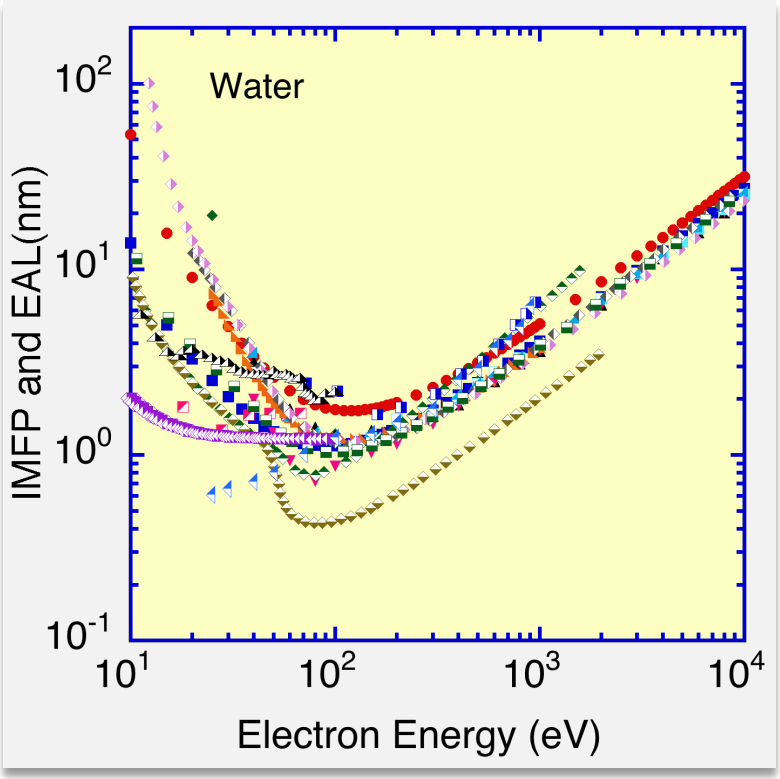
$$\lambda = \frac{E}{E_p^2 \beta \ln(\gamma E)}$$

4. IMFPs and EALs in liquid water

: evaluation of ELF at q>0

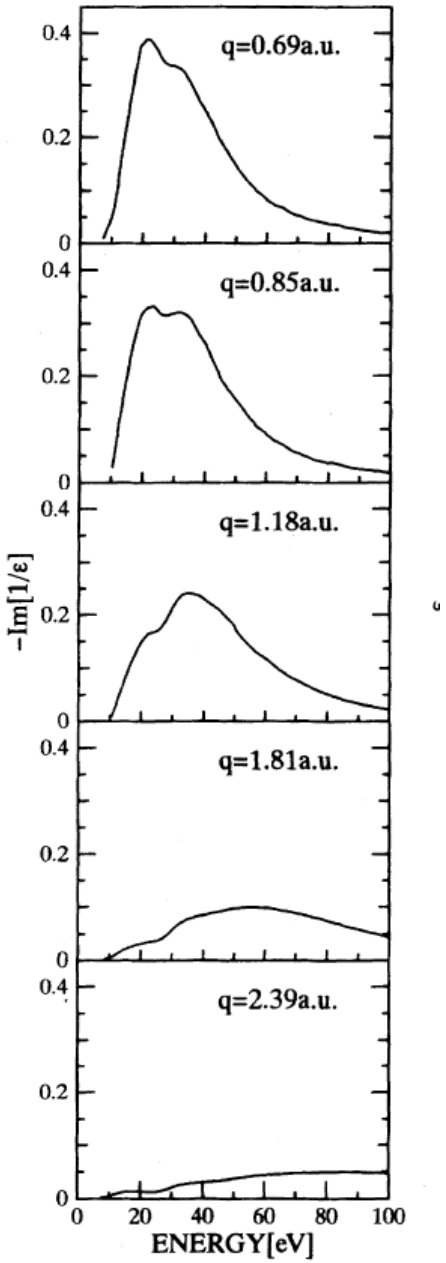
- important to know details of the interactions of low-energy electron with liquid water for many biological applications, especially for the investigation of cellular and sub-cellular dosimetry

- Inelastic mean free path (IMFP) : good measure
  most basic physical quantity



- many studies to determine the IMFPs and EALs in water
- but large variations in IMFP and EAL values
- mainly due to the calculation algorithm and the energy-loss function (ELF) used for the IMFP calculations.

Evaluation of ELFs at q >0



- Hayashi et. al reported ELFs of water at 3.59 ≥q≥0.69 that were determined with **Inelastic X-Ray scattering spectroscopy (IXSS).**
(Bull. Chem. Soc. Jpn.**,70**, 719 (1997))

- Also reported the static structure factor *S(q)*

$$S(q) = \int_0^\infty S(q,E)\,dE = \int_0^\infty \frac{\hbar (q a_0)^2}{4\pi^2 e^2 n} \mathrm{Im}\left(\frac{-1}{\varepsilon(q,E)}\right) dE$$

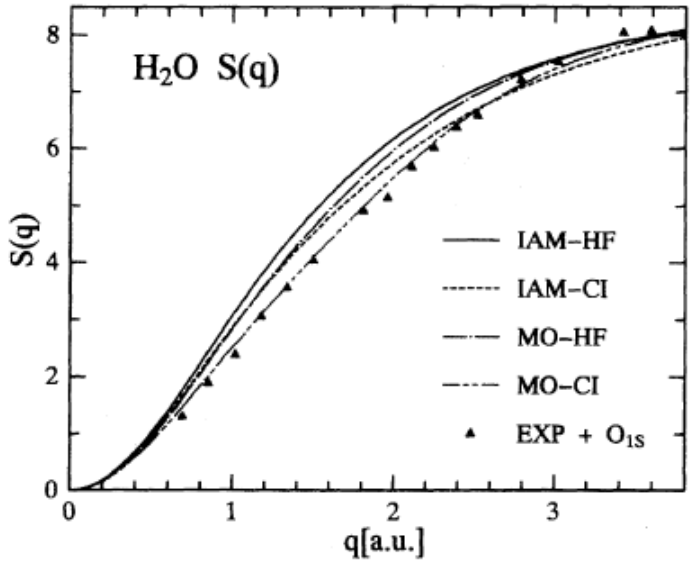
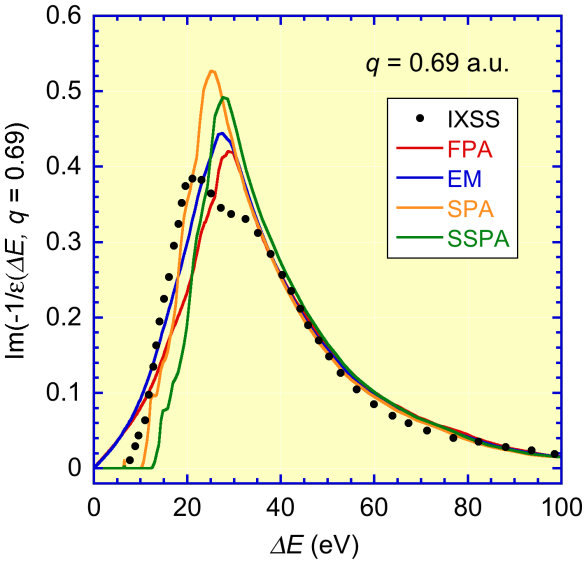
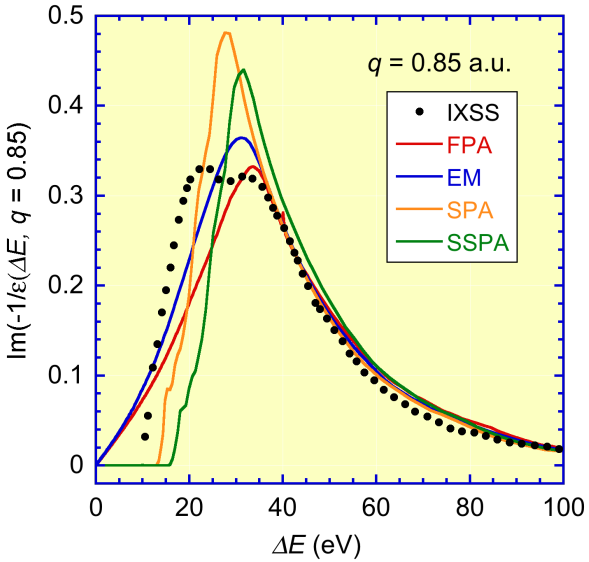


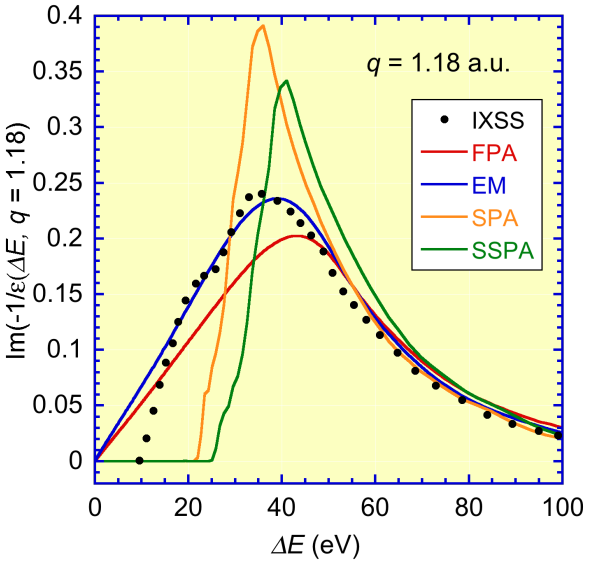
Fig. 7. A comparison of the observed $S(q)$'s with various calculations.

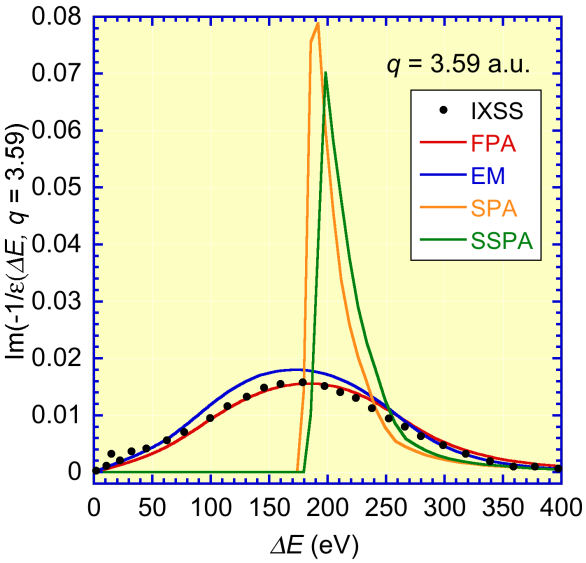
- good measure for evaluate ELFs at q>0 that can be calculated by various algorithms

Comparison of the experimental ELF of liquid water for q = 0.69, 0.85, 1.18 and 3.59 a.u.





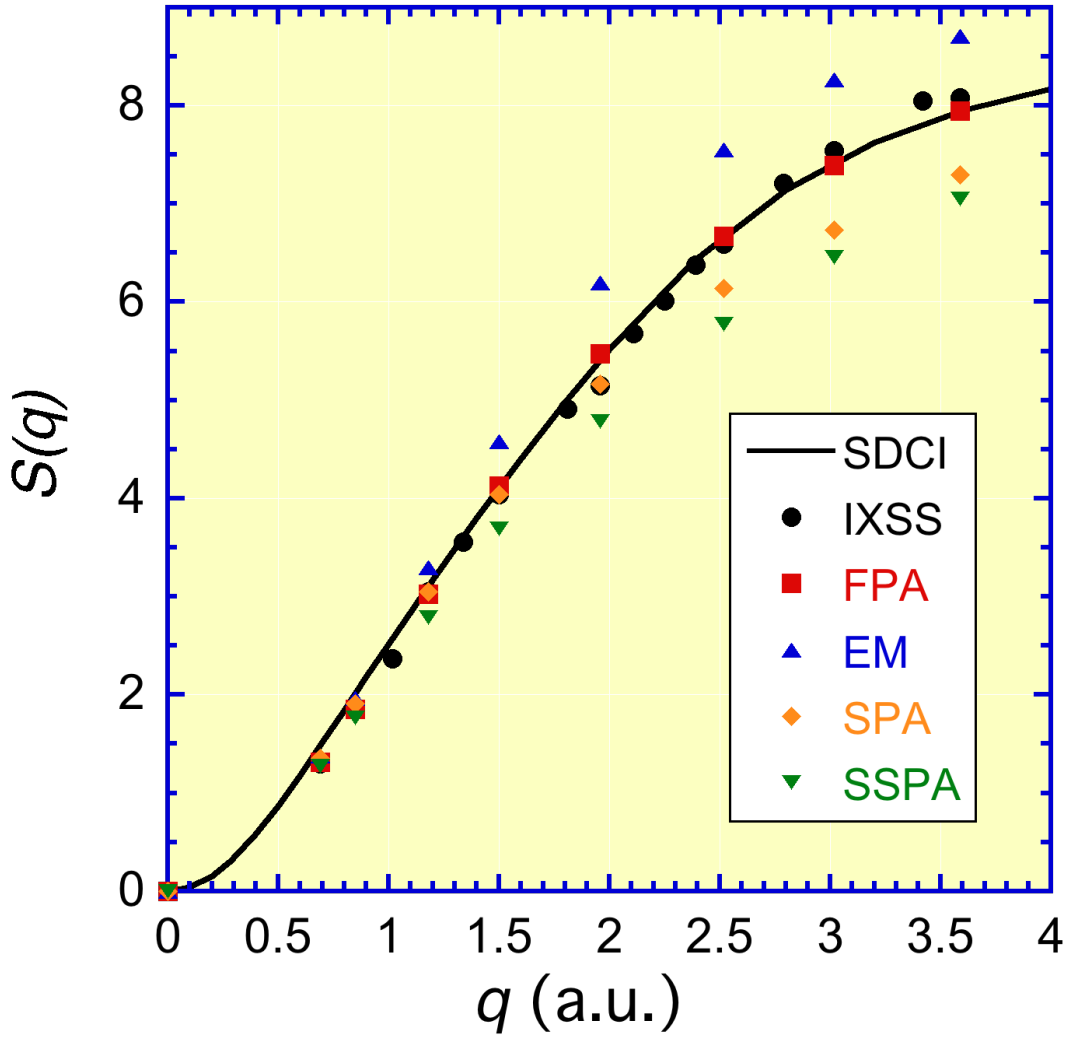




The solid circles represent the measured ELF with inelastic X-ray scattering spectroscopy (IXSS) by Hayashi *et al*. .

The solid lines shows the ELF at q obtained from FPA, EM, SPA , and SSPA from ELF at q=0

Plots of the static structure factor S(*q*) of water as a function of momentum transfer *q*



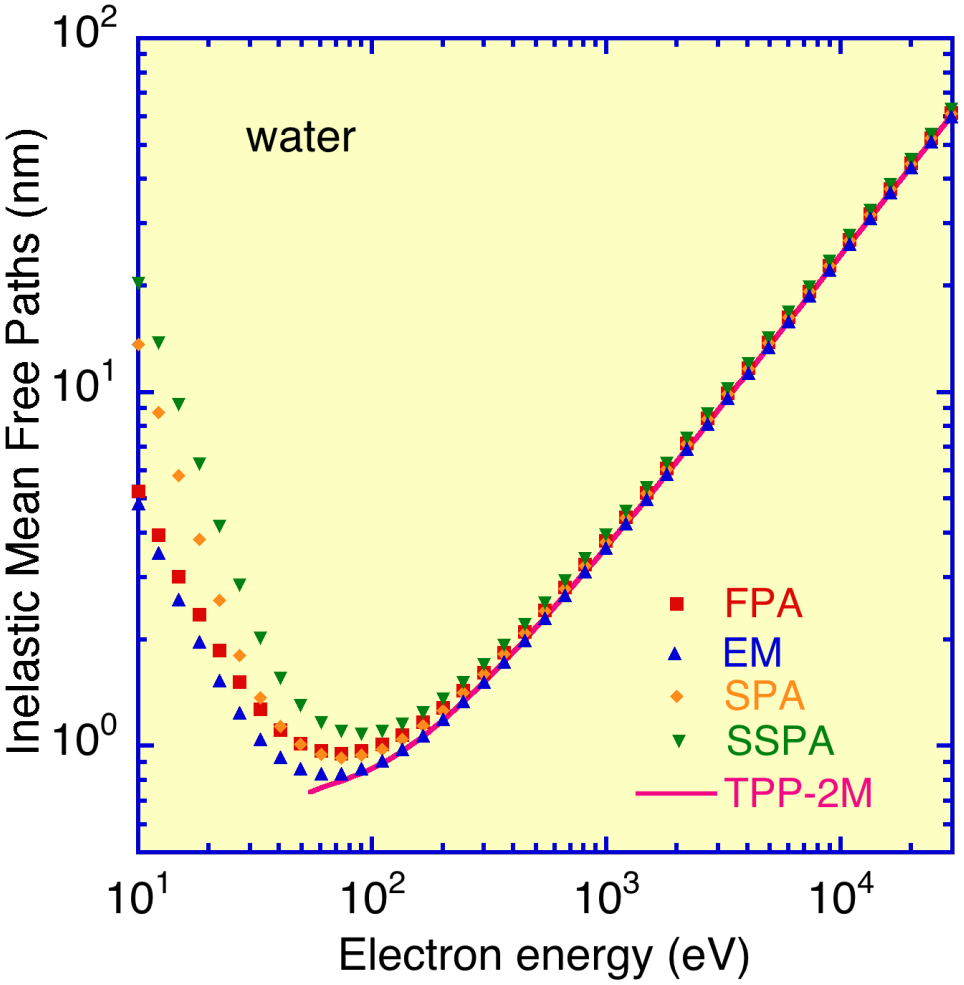
- SDCI :first-principle calculations with configuration iteration (CI) wave functions including all single and double excitations.
- IXSS: measured value

$$S(q) = \int_0^\infty S(q,E)\,dE = \int_0^\infty \frac{\hbar (q a_0)^2}{4\pi^2 e^2 n} \mathrm{Im}\left(\frac{-1}{\varepsilon(q,E)}\right) dE$$

- calculated from ELF at q=0 with various algorithm

- S(*q*) is a good measure to evaluate the algorithm for IMFP calculation

IMFP for water from optical $ELF_{q=0}$



$$\lambda = \frac{\alpha(T)T}{E_p^{\,2}\left\{\beta_{nr}\left[\ln\left(\gamma_{nr}\alpha(T)T\right)\right] - C/T + D/T^2\right\}}$$

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

$$\gamma_{nr} = 0.191\rho^{-0.5} \qquad (\mathrm{eV^{-1}})$$

$$C = 19.7 - 9.1U \qquad (\mathrm{nm^{-1}})$$

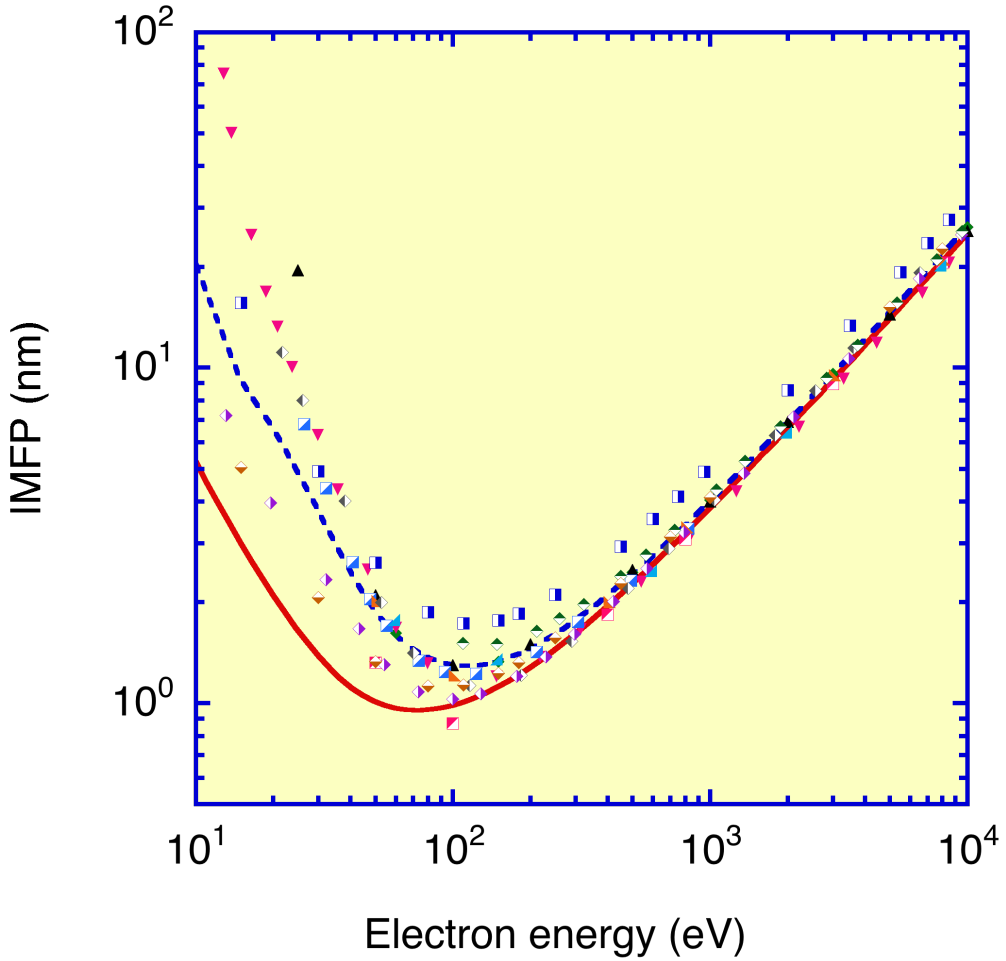
$$D = 534 - 208U \qquad (\mathrm{eVnm^{-1}})$$

$$U = \frac{N_v\rho}{M} = \left(E_p/28.816\right)^2$$

50 – 30,000 eV : IMFPs of TPP-2M
good agreement (RMS 7.9 % for FPA)
> 200 eV : RMS 4.6% for FPA

EM: RMS 2.4% 50 – 30, 000 eV

Comparison : other IMFPs calculated



FPA : $\omega_{max} = T - E_f$

SSPA DA : $\omega_{max} = \min [T - E_f, T/2]$

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

Simplified SPA: $\omega_{max} = T/2$

- Ashley et al., Tung et al.
- Tomita et al., Akkerman
- Dingfelder et al.

$$\mathrm{Im}\left[\frac{-1}{\varepsilon(q,\omega)}\right] = \frac{\omega_0}{\omega}\mathrm{Im}\left[\frac{-1}{\varepsilon(\omega_0)}\right],$$

$$\omega_q(\omega_p) = \omega_p + \frac{q^2}{2}.$$

12 Emifietzoglou $E_i(q) = E_i + g(q)\frac{q^2}{2m_e}$

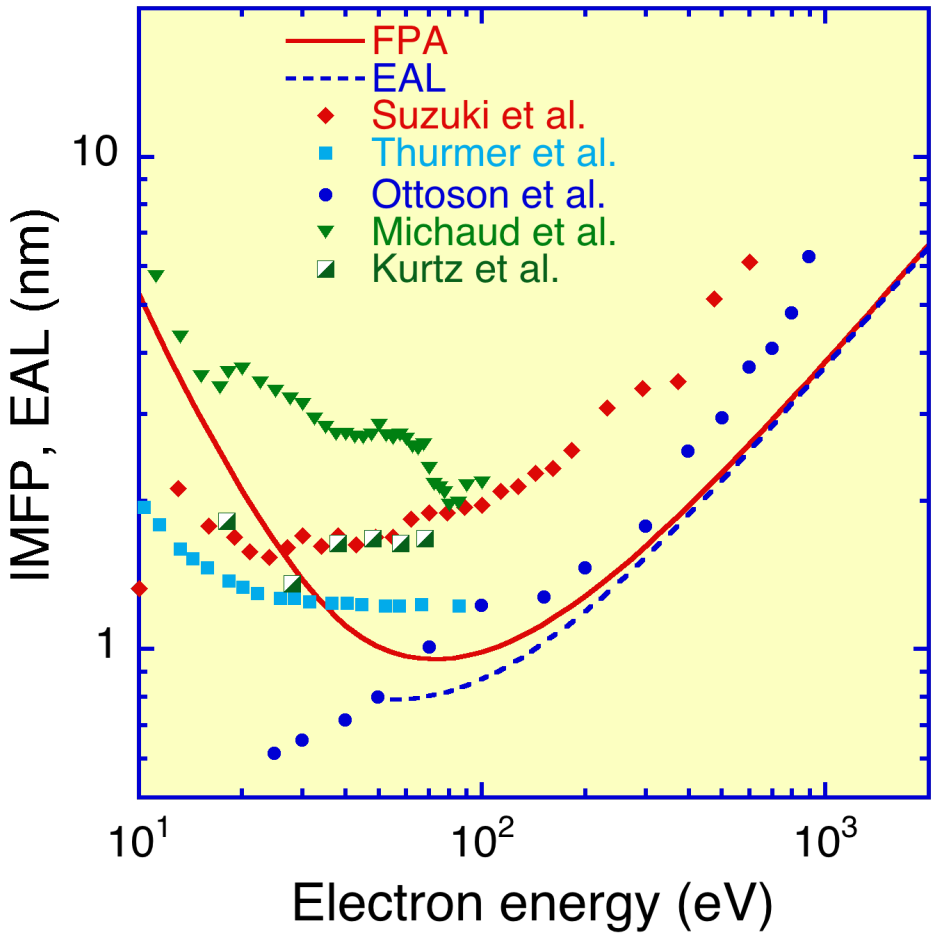
where $g(q) = 1 - \exp(-cq^d)$ and

$\gamma_i(q) = \gamma_i + aq + bq^2$

13 Emifietzoglou

- XC including static and dynamic LFC

Comparison : measured EALs



EAL: Jablonski-Powell eq. using FPA-IMFP values.

$$L = \lambda(1 - 0.735\omega) = \lambda\left[1 - 0.735\left(\frac{\lambda}{\lambda + \lambda_{tr}}\right)\right]$$

Kurtz et al.: condensed films of water ice.

Michaud et al. : amorphous ice ; HREELS.

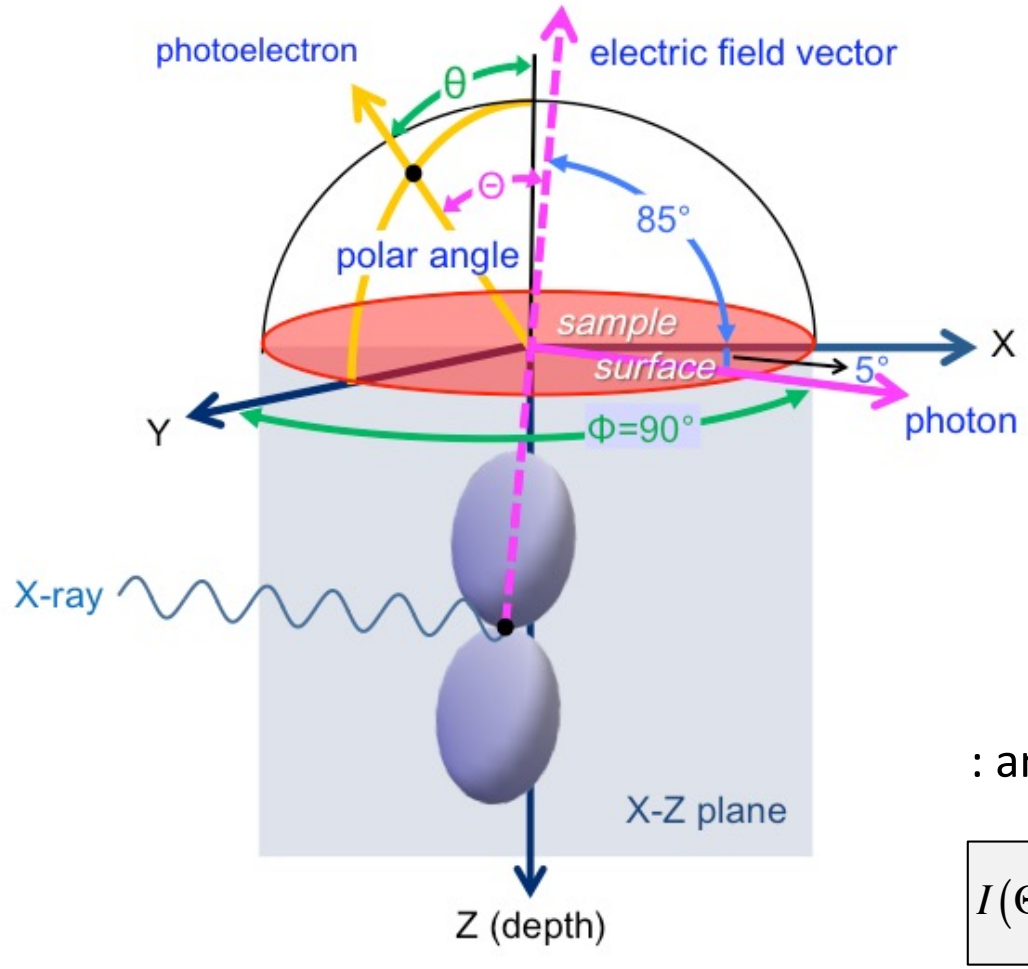
Ottoson et al.: liquid water; a liquid micro-jet in combination with soft X-ray SR.

Thurmer et al.: IMFPs ; PE angular distribution + ELAs of Ottoson.

Suzuki et al.: liquid water ; soft x-ray O1s photoemission spectroscopy of a liquid beam of water without any theoretical estimation.

5. Calculation of MED for HAXPES

- MEDs of PEs excited by linearly polarized X-rays



Schematic diagram of the experimental configuration for Monte Carlo calculations

- **X-ray incident angle : 85°**
- **Emission angle : θ = 0° - 80°** (10° st
- **Azimuthal angle: Φ = 90° , 0°**

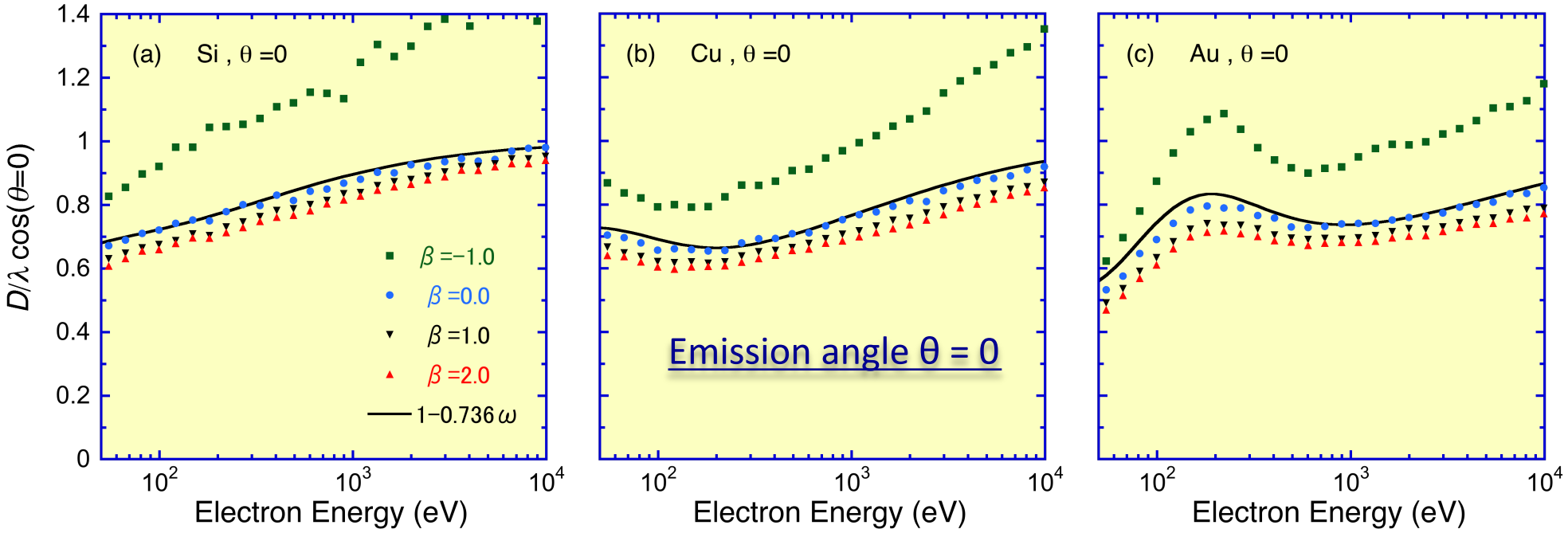
- PE kinetic energy : 50 eV – 10keV
- β = -1 to 2 (0.5 step)
  γ = 0, δ = 0 (multi-pole)

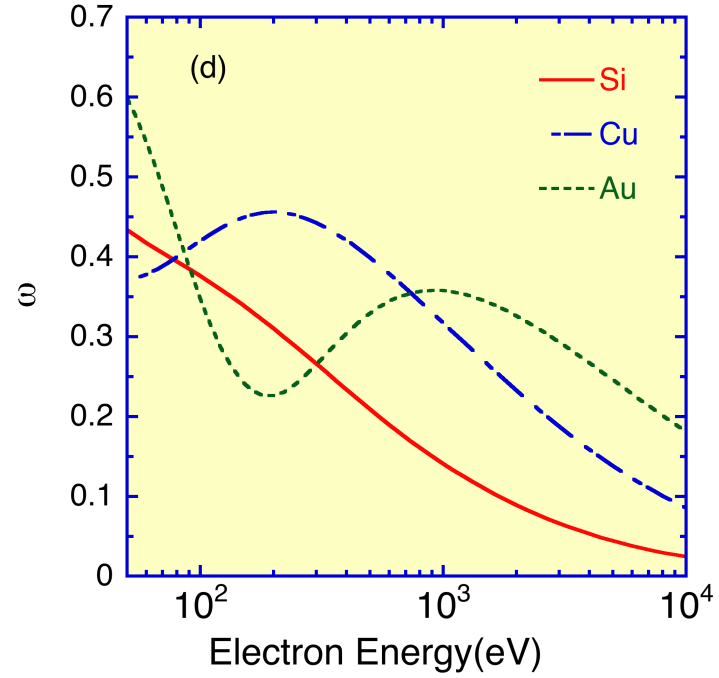
: angular distribution of PEs

$$I(\Theta)=\frac{\sigma}{4\pi}\left[1+\frac{\beta}{2}\left(3\cos^2\Theta-1\right)\right]$$

$$I(\Theta)=\frac{\sigma}{4\pi}\left[1+\frac{\beta}{2}\left(3\cos^2\Theta-1\right)+\left(\gamma\cos^2\Theta+\delta\right)\sin\Theta\cos\Phi\right]$$

3. Analysis of MED: **Dependence on Electron Energy**





Jablonski-Powell equation

$$\frac{D}{\lambda\cos(\theta=0)} = 1 - 0.736\omega$$

- good guide in wide energy range
- slightly larger than MC results (β ≥ 0)

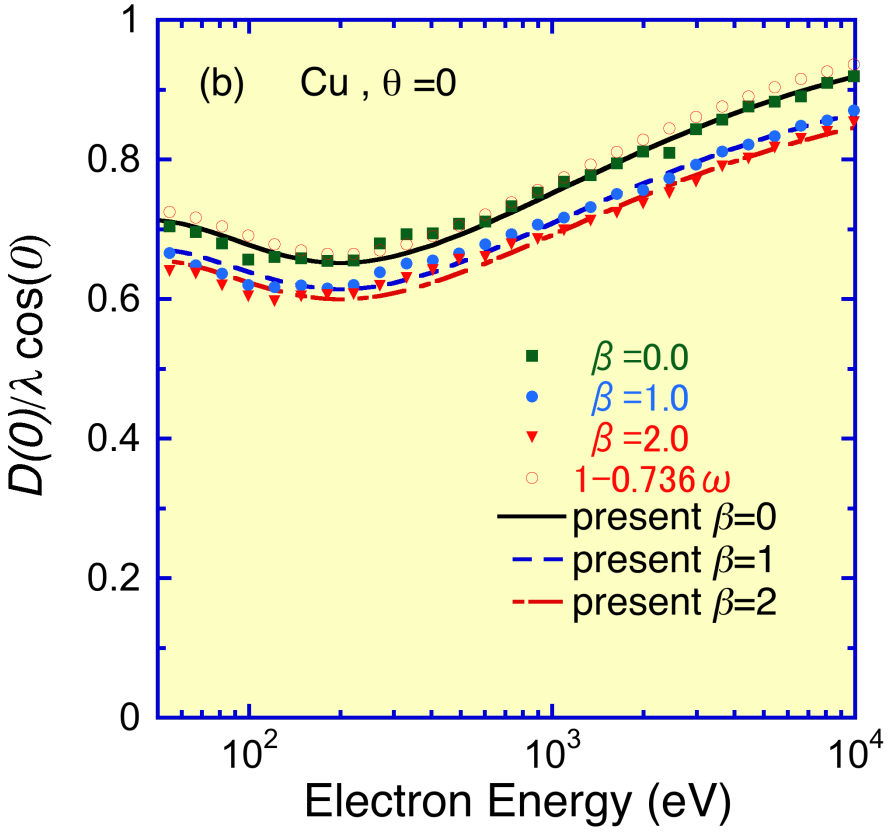
- no β dependence

Resulting MED equation for Linearly Polarized X-ray

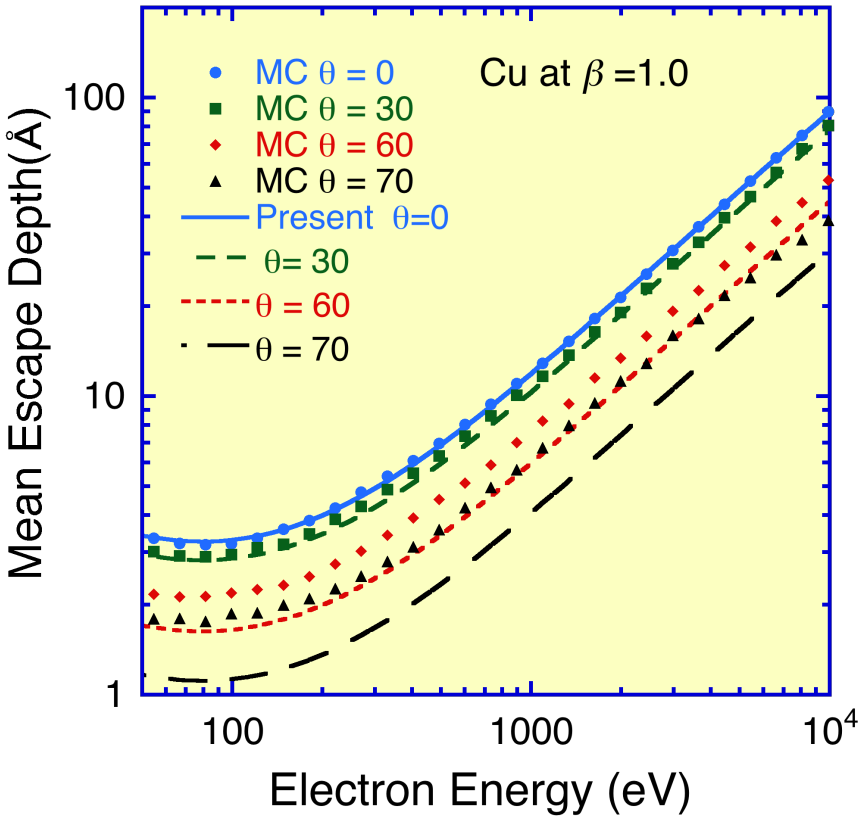
$$D(E,\theta,\beta,\lambda,\omega) = g(\beta)\times 0.981(1-0.736\omega)\lambda\cos\theta$$

$$g(\beta) = 1.00 - 0.102\beta + 0.0577\beta^2 - 0.0133\beta^3$$

Energy range : 100 eV – 10 000 eV
Emission angle : 0° ≤ θ ≤ 40°
Asymmetry parameter: -0.5 ≤ β ≤ 2.0

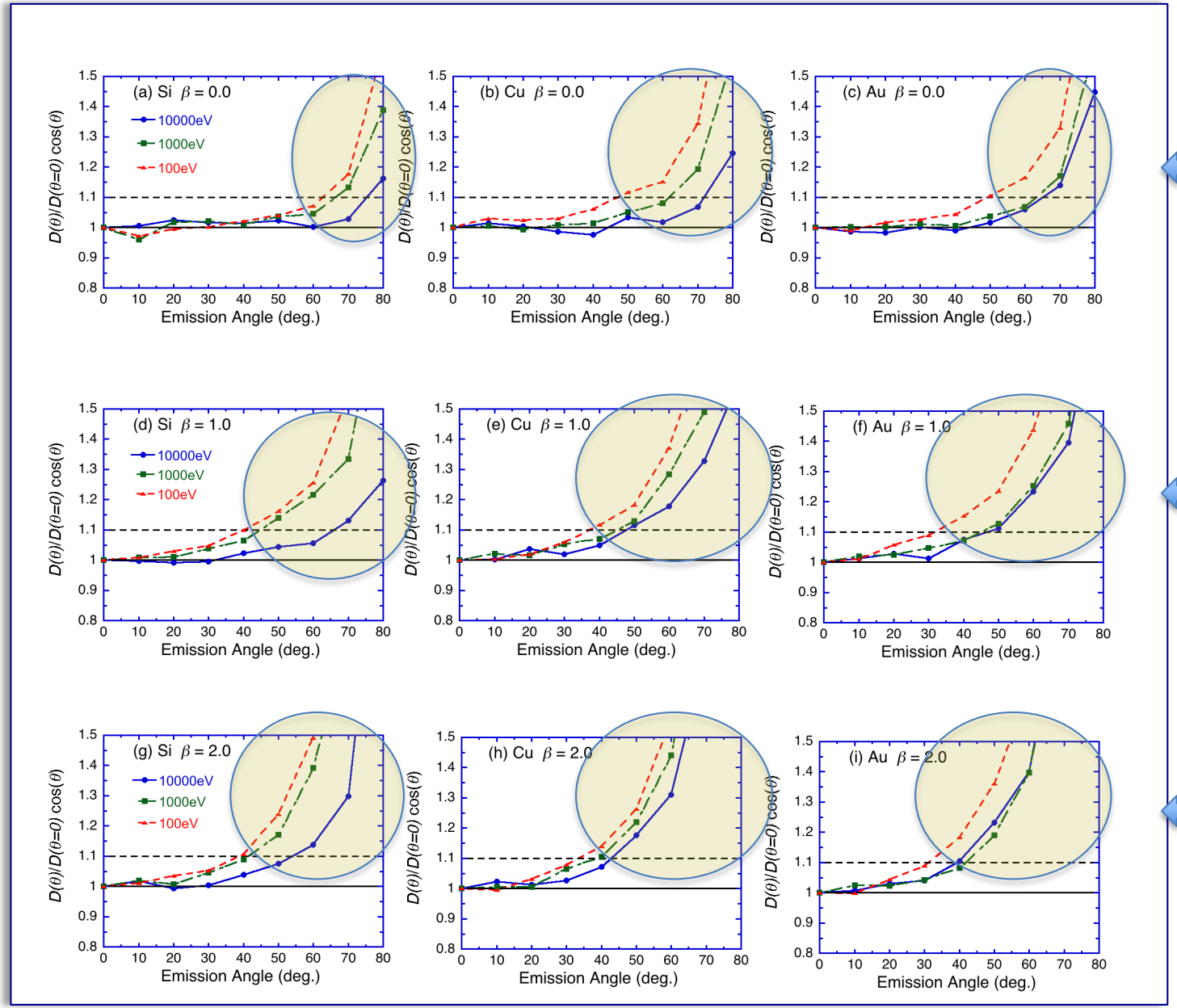


- MED on β dependence at θ=0



- MED on θ dependence at β=1

Normalized MED , D(θ)/D(0) cos(θ) vs. emission angle θ



β=0

: ≥1000 eV
θ≤60°
:100 eV
θ≤50°

β=1

: ≥1000 eV
θ≤45°
:100 eV
θ≤30°

β=2

: ≥1000 eV
θ≤40°
:100 eV
θ≤30°

6. Summary

- We calculated IMFPs for 41 elemental solids and 42 inorganic compounds 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 : 0.7% for elemental solids, 0.6% for inorganic compounds.

- **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)

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.**

Summary-3

- MEDs of PEs excited by linearly polarized X-rays in Si, Cu, and Au over the 50 to 10,000 eV. (MC method)
- MED values increase as the β values decrease over the 50 to 10,000 eV .
- Energy dependences of the ratios $D/\lambda\cos(\theta)$ *at* $\theta=0$ can be expressed by the form of Jablonski-Powell predictive equation , which is a function of single-scattering albedo, over 50 eV to 10,000 eV.
- $D(\theta)/D(0)\cos\theta$ are approximately constant to within 10% for
  - $0^\circ \le \theta \le 40^\circ$, $-0.5 \le \beta \le 2.0$, and $E \ge 1000$ eV

  ($0^\circ \le \theta \le 60^\circ$, $\beta = 0$, and $E \ge 1000$ eV)

: a simple predictive MED equation that could be applied to the wide energy range and dipole parameter that are used in high-energy XPS with synchrotron radiation.

These works were performed in collaboration with

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

H. Yoshikawa (NIMS) : REELS- FA, MEDs

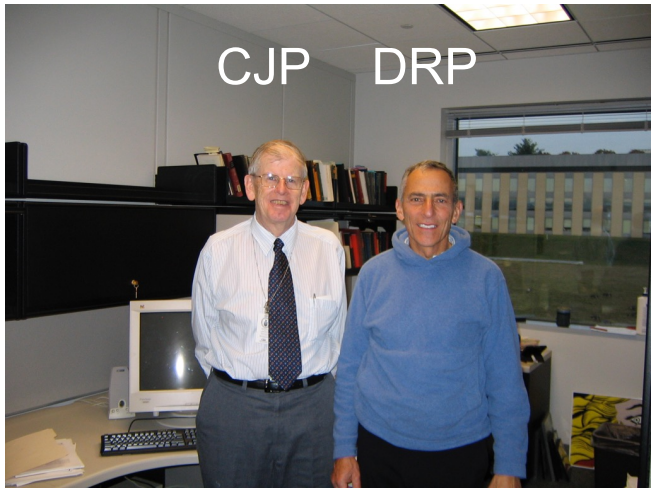
K. Goto (NIT, AIST) : EPI measurements

R. Ueda (NIMS) : MEDs

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

B. Da (NIMS) : EM (super EM method)

Jun. 1987



Nov. 2004

Jun. 2013

Thank you for your attention !