# Determination of Inelastic Mean Free Paths in Elemental Solids in the 200 to 5000 eV Energy Range by Absolute Elastic Peak Electron Spectroscopy

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- Introduction
- Measurement of EPI
  - Comparison of measured and calculated EPI
- IMFP determination
  - Comparison of measured and calculated IMFPs
    ( TPP-2M and from ELFs)
- Analysis of IMFPs determined from EPIs by Fano Plots
  - comparison of EPES with Ni-std method
- Summary

# 1. Introduction

- Knowledge of the values of inelastic mean free paths (IMFPs) for low-energy electrons in solids is important for quantitative surface analysis by AES, XPS, and EELS.

**: We have determined IMFPs for Ag, Au, Cr, Cu, Fe, Ga, C (Graphite) , Mo,Ni, Pt, Si, Ta, W and Zn in the 50 - 5000 eV energy range from Absolute backscattered elastic-peak intensities and compared with the corresponding calculated IMFPs ( optical and TPP-2M ) in order to check their reliability.**
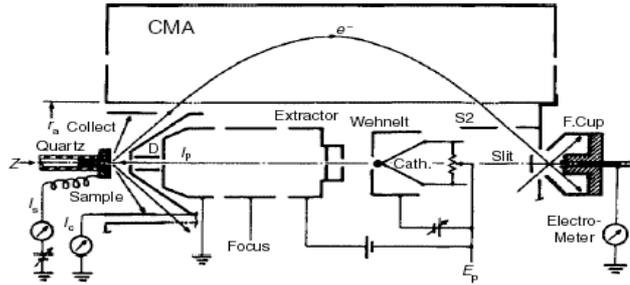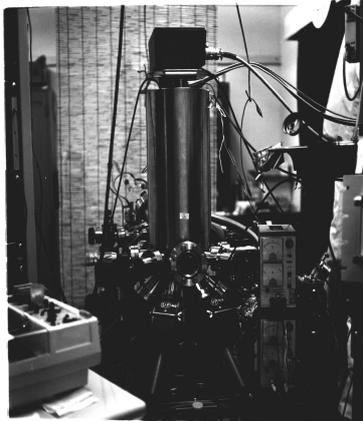
# Measurements of EPIs



Figure 1. Schematic CMA system.

CMA $\Delta E/E = 0.25\%$

Accuracy
$\pm$ 0.01% (primary beam energy)
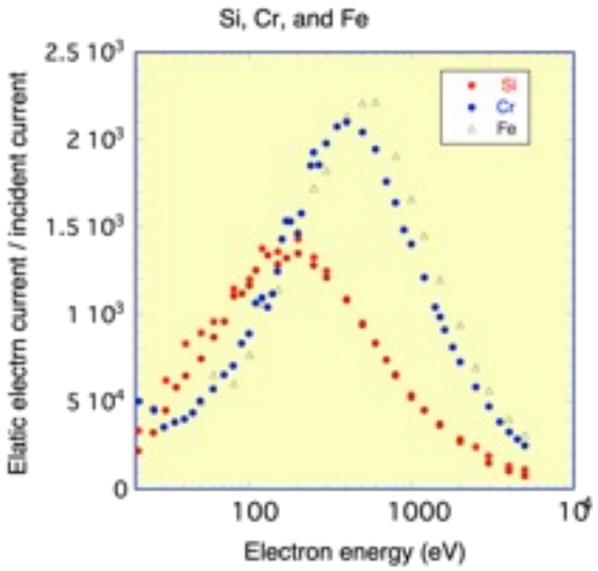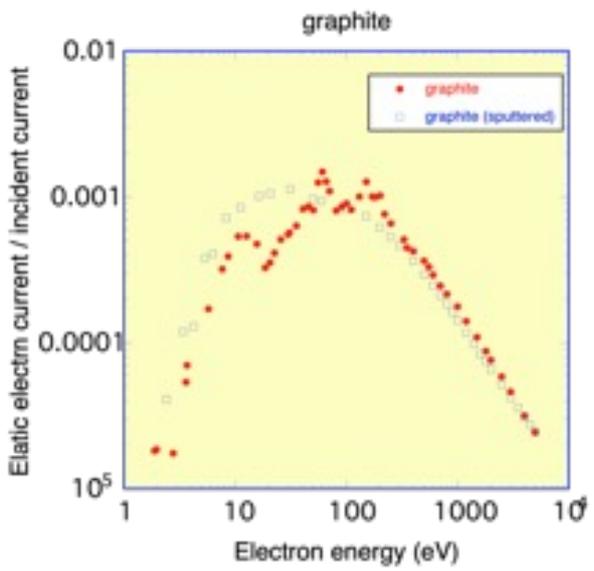$\pm$ 0.5% (Auger spectra)

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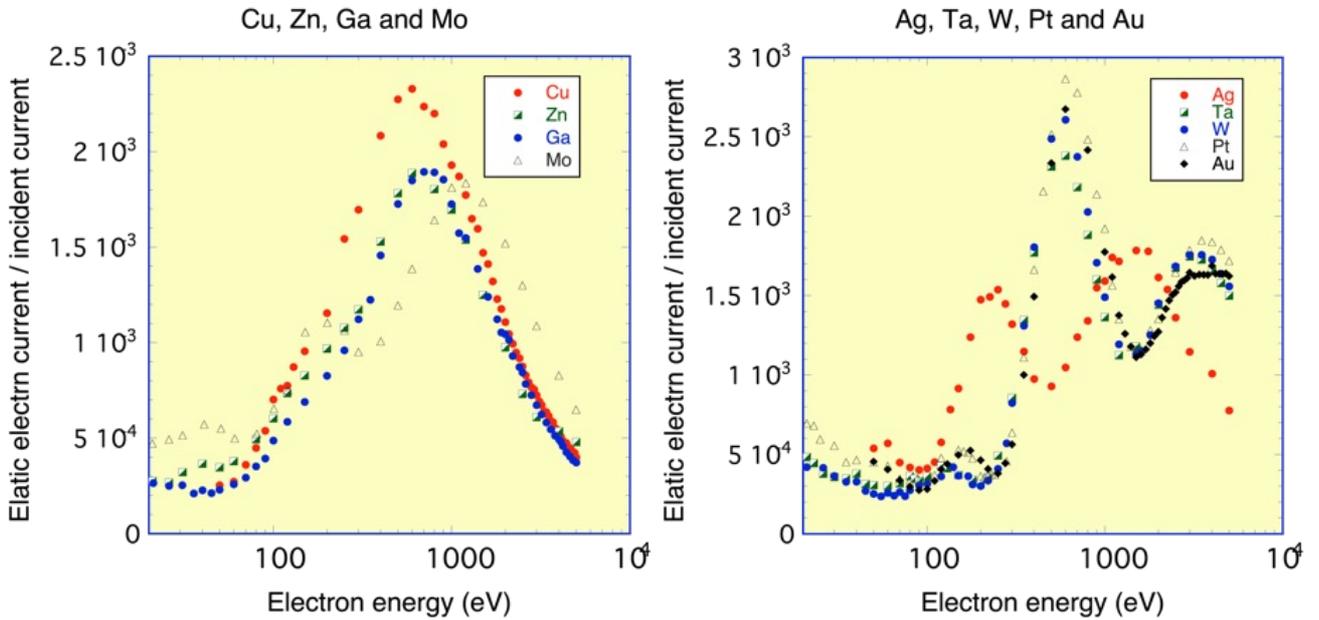  -detection angle (42.3$\pm$ 6°)

Primary beam: 1 $\mu$A
Detector: Faraday cup

3

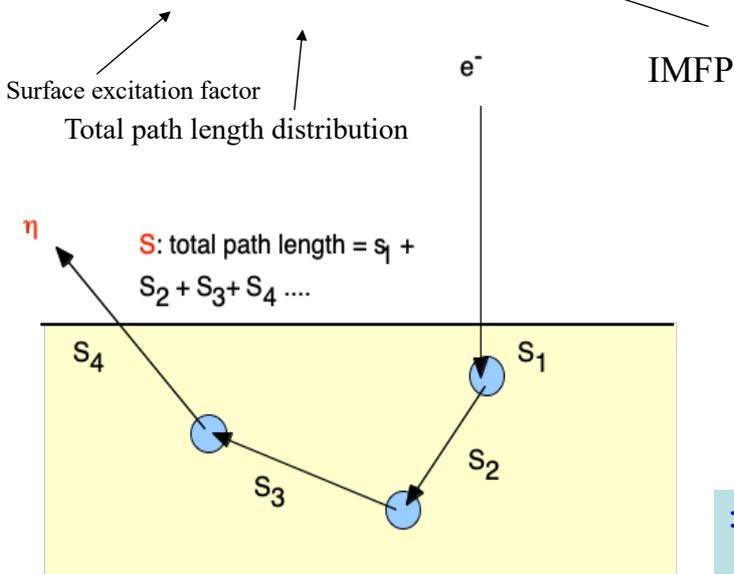# Measured elastic peak intensity as a function of electron energy  -1



4

# Measured elastic peak intensity as a function of electron energy -2



Cu, Zn, Ga and Mo



Ag, Ta, W, Pt and Au

# Calculation of EPIs with MC method

$$\frac{I}{I_0} = G_w \times G_t \times f_S \int_0^\infty \left(\frac{d\eta}{dS}\right)/N_0 \exp\left(-\frac{S}{\lambda}\right) dS$$
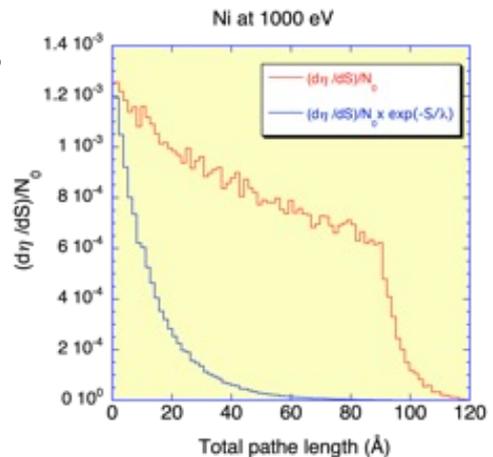
Surface excitation factor

Total path length distribution

$e^-$

IMFP

$G_t$ : transmission efficiency of CMA

$I_0$ : incident electron current

$N_0$ : number of input elctrons

Ni at 1000 eV



η

S: total path length = $s_1$ + $s_2$ + $s_3$ + $s_4$ ....

$S_4$   $S_1$
$S_3$   $S_2$

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

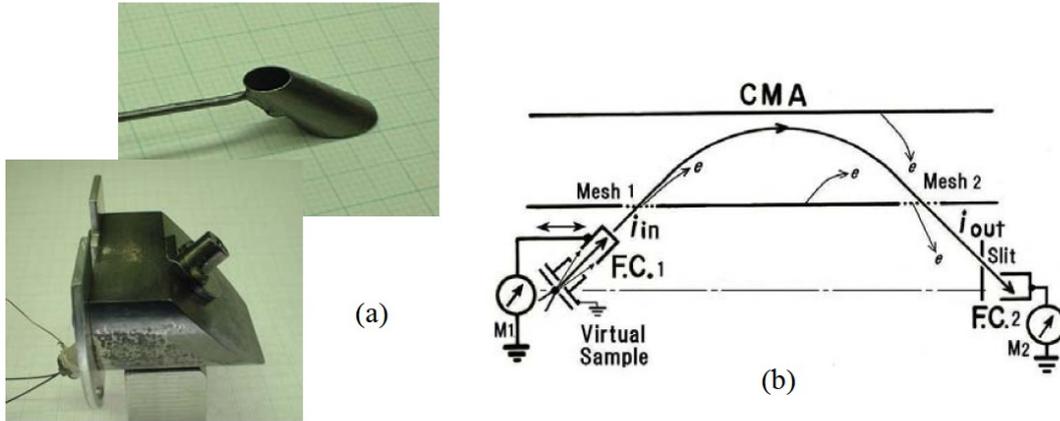Gw : correction for window in CMA

Fig. 1. (a) Virtual Sample and F.C.1 photos. (b) Schematic experimental set up.
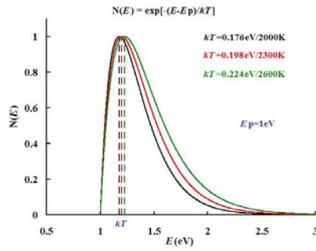
# Simulation of $G_t$

**Simulation results:**



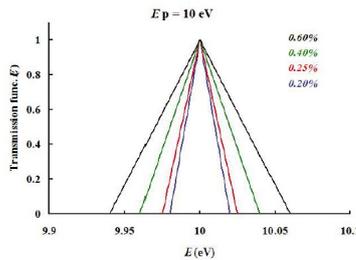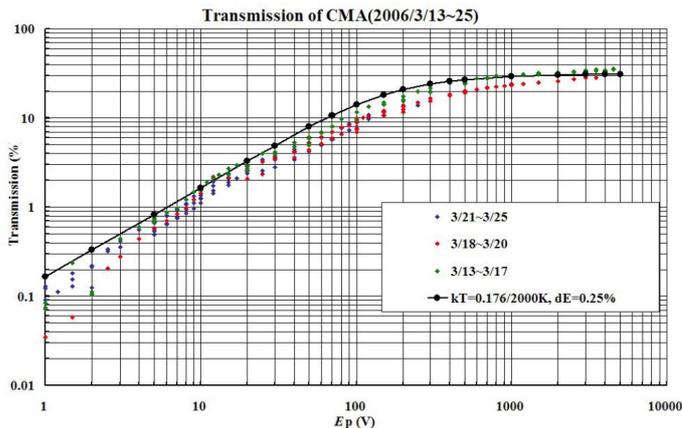Fig.2. Thermal emitted electrons function for different values of $T$. for the acceleration of $E$p=1V.

Fig.3. Energy transmission function for different values of $\Delta E/E$. (case for $E$p=10eV)

# Comparison of measured and calculated EPIs for Au in the 50 - 5000 eV



Au
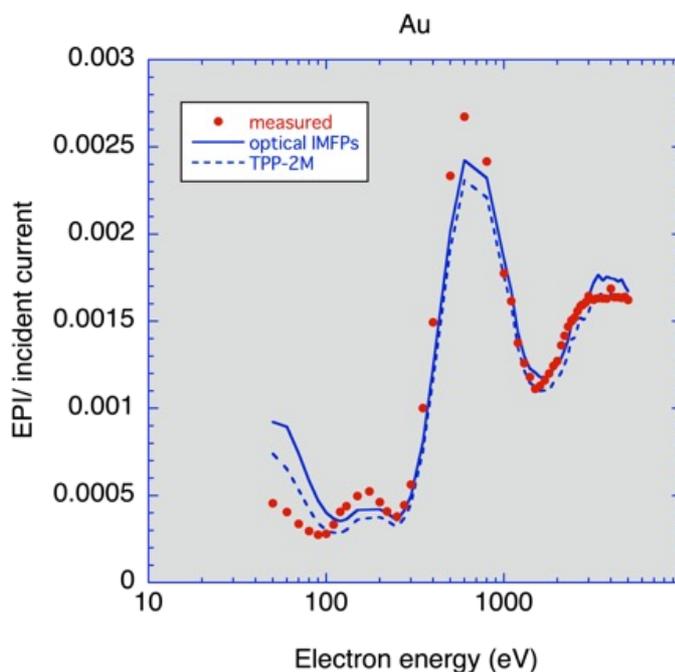
Measured intensity
- solid circles: EP current /incident

Calculated intensities from MC method (without fs correction)
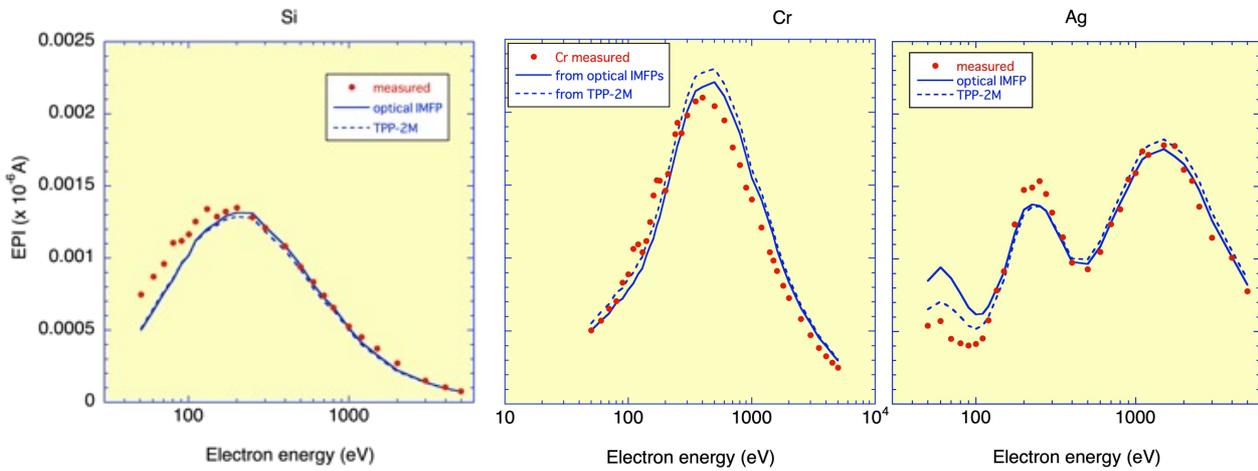- solid line ( optical IMFPs)
- dotted line ( TPP-2M)

$$\left(\frac{I^{\mathrm{x}}}{I_0}\right)_{\mathrm{cal}} = G_{\mathrm{w}} \times G_{\mathrm{t}} \times f_{\mathrm{S}} \int_0^\infty \left(\frac{d\eta}{dS}\right)^{\mathrm{x}} / N_0 \exp\left(-\frac{S}{\lambda_{\mathrm{x}}}\right) dS$$

$$f_S = 1$$

200eV >    : good agreement

200 eV<    : large diffirence

10

## Comparison of measured and calculated EPIs of Ag, Si and Cu in the 50 - 5000 eV

## Determination of IMFPs from Absolute EPIs

: Measured EPI

$$\left(\frac{I^x}{I_0}\right)_{measured} : \quad I^x \to EPI \quad I_0 = 10^{-6}A$$

: Calculated EPI with MC  (parameter $\lambda_x$ (IMFP))

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

: IMFP determination

$$\left|\left(\frac{I^x}{I_0}\right)_{measured} - G_w \times G_t \times f_S \int_0^\infty \left(\frac{d\eta}{ds}\right)^x / N_0 \exp\left(-\frac{s}{\lambda_x}\right) dS\right| \to \min$$
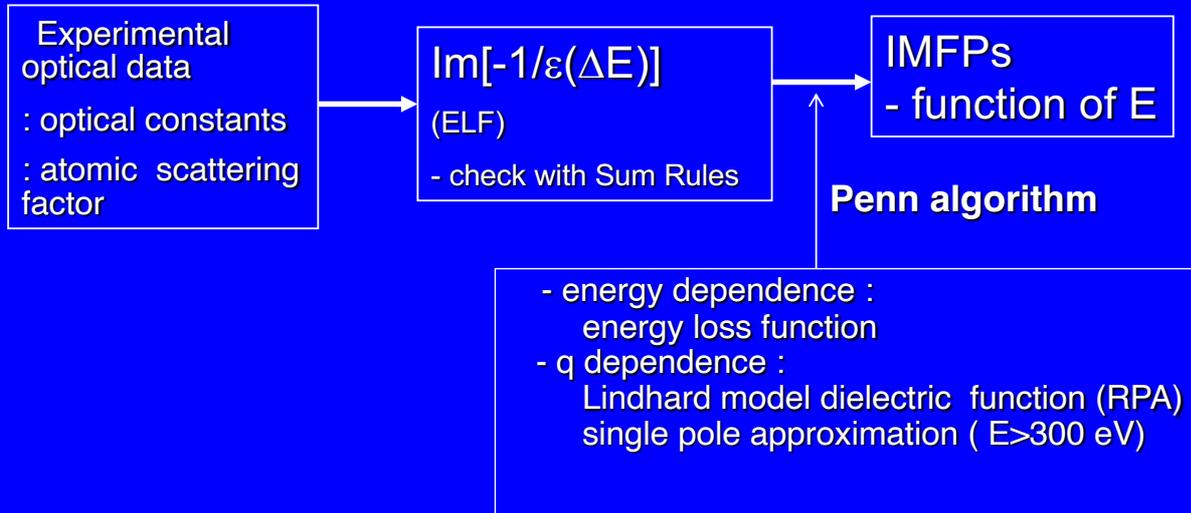
- solve above eq. for parameter $\lambda_x$ (IMFP)

# Calculation of IMFPs from optical data (Optical IMFPs)

• Flow of calculation

$$\frac{d^2\sigma}{dqd\omega} = \frac{me_0^2}{\pi NhE}\,\mathrm{Im}\!\left(\frac{-1}{\varepsilon(q,\omega)}\right)\frac{1}{q}$$

$$n\sigma\lambda = 1$$

Experimental optical data

: optical constants

: atomic scattering factor

→

Im[-1/ε(ΔE)]

(ELF)

- check with Sum Rules

→

IMFPs
- function of E

**Penn algorithm**

- energy dependence :
   energy loss function
- q dependence :
   Lindhard model dielectric function (RPA)
   single pole approximation ( E>300 eV)

13

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# TPP-2M

$$\lambda = \frac{E}{E_p^2\left[\beta \ln(\gamma E) - CE^{-1} + DE^{-2}\right]} \quad\text{(A)}$$

$$\beta = -0.10 + 0.944\left(E_p^2 + E_g^2\right)^{-0.5} + 0.069\rho^{0.1}$$

$$\gamma = 0.191\rho^{-0.5}$$

$$C = 1.97 - 0.91U$$

$$D = 534 - 208U$$

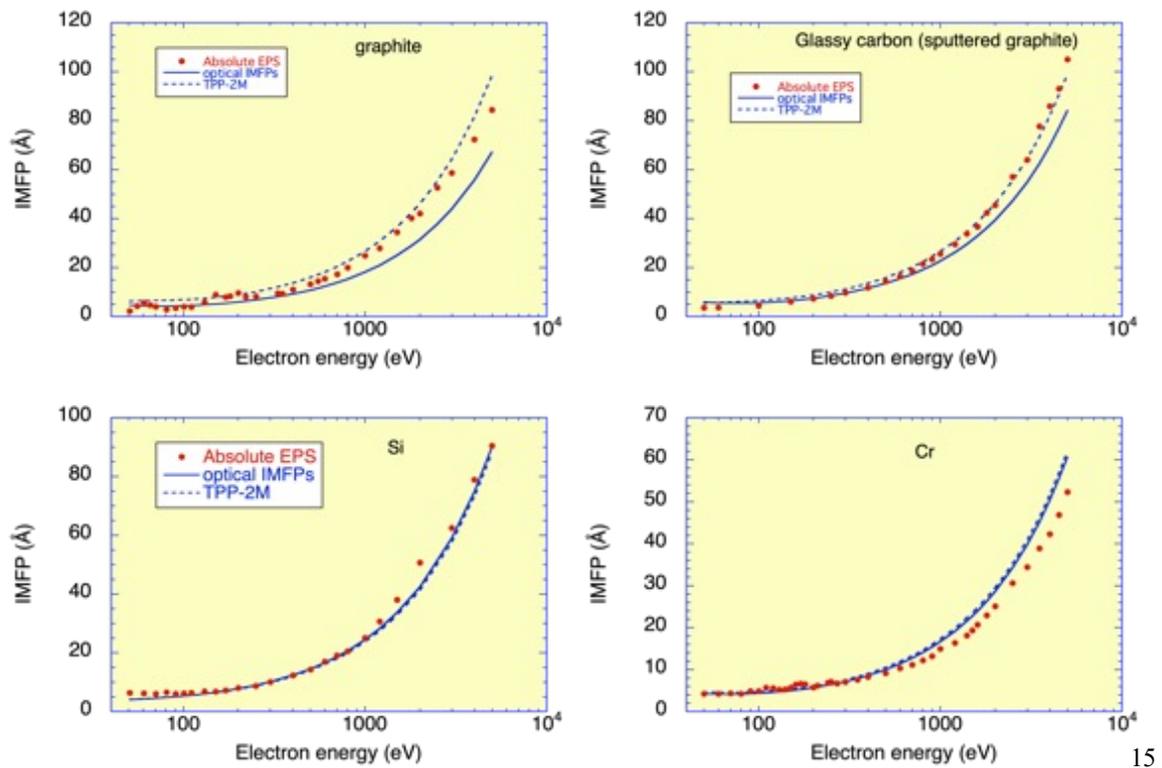$$U = \frac{N_v\rho}{M} = \frac{E_p^2}{8294}$$

M: atomic weight

ρ: density

Nv: number of valence electrons
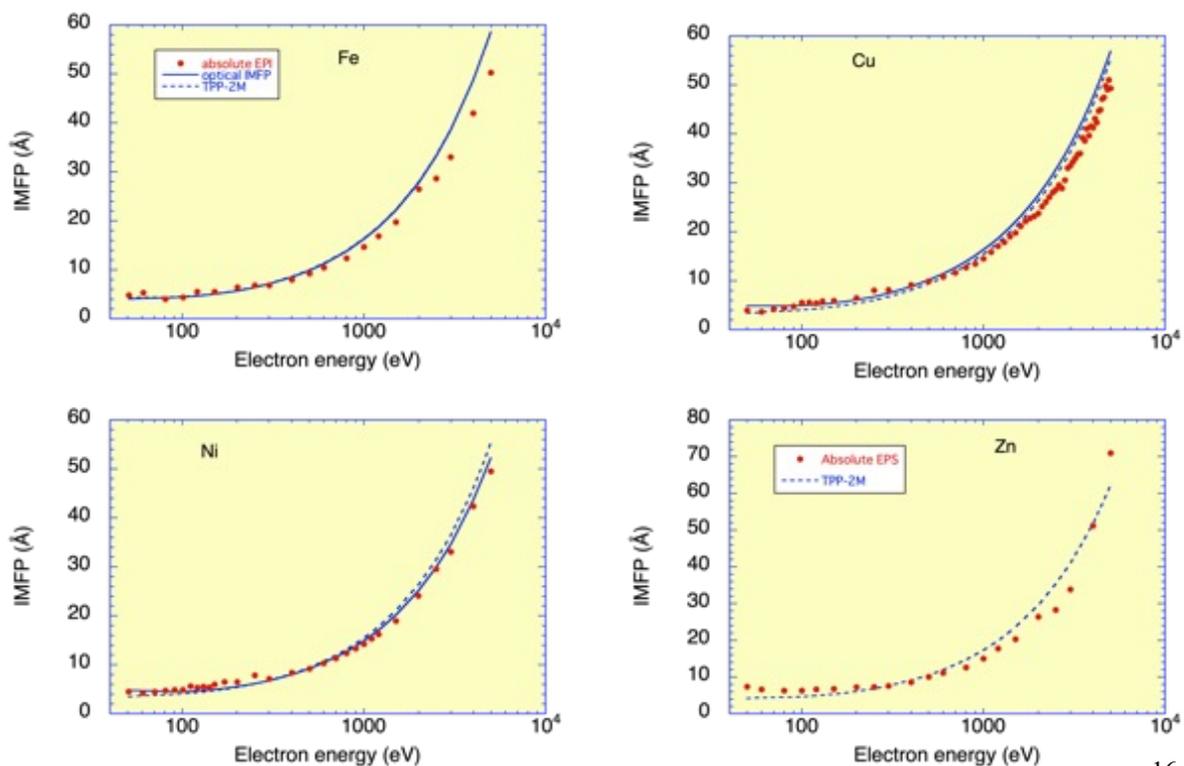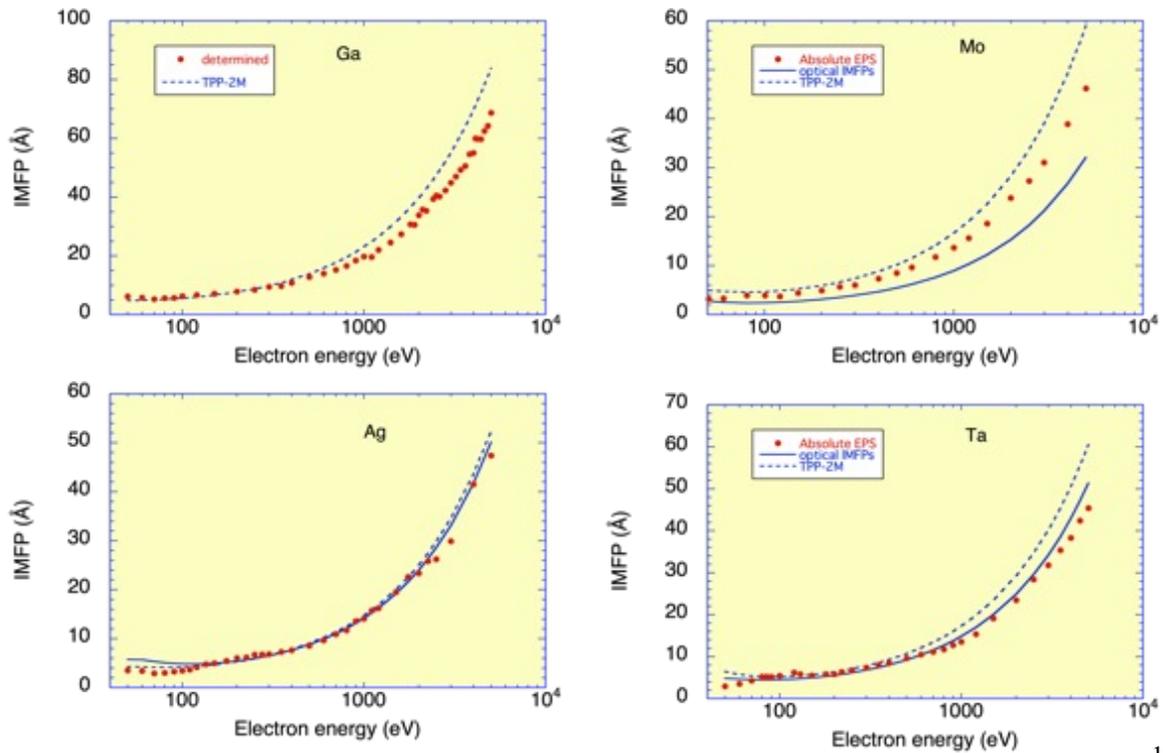
Eg: band-gap energy

14

# IMFPs determined from Absolute EPI
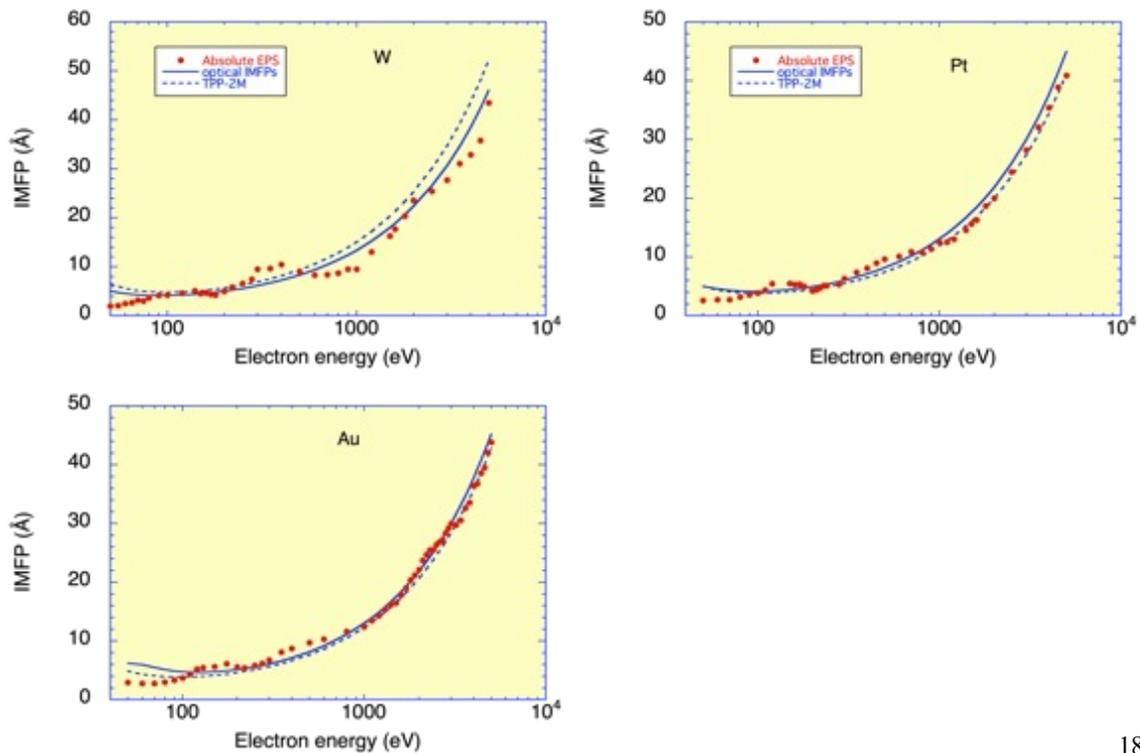


15

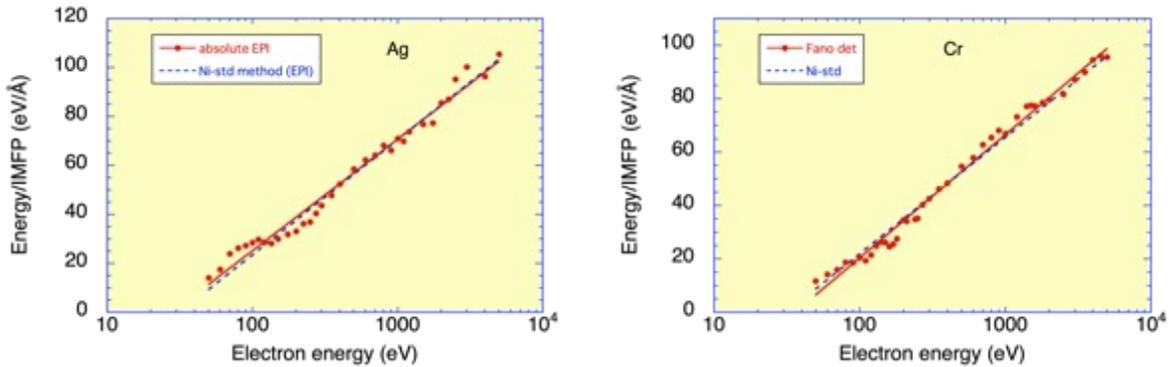# IMFPs determined from absolute EPI



16

17

# IMFPs determined from absolute EPI



18

# Analysis of IMFPs with Fano Plot

- We have analyzed experimentally determined IMFPs using Fano Plots
which were constructed by plotting values of E/λ *versus* ln E.



solid symbols :experimentally determined IMFPs

red solid line: fit to the energy/IMFP values with the Bethe equation

   dotted line: calculated from Bethe equation (experimental IMFP value: EPES-Ni-std )

$$E/\lambda = E_p^2 \beta \ln(\gamma E)$$   ⟸   Simple Bethe equation

19

# Dotted line: IMFPs from EPIs using Ni-std

- Calculation of EPI ratio to Ni-reference    ;  remove $G_t$

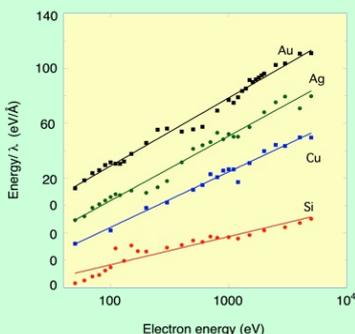$$f_s^x / f_s^{Ni} = 1$$   - assume that  surface excitation  effect is negligible for Ni-reference method.

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

Determination of IMFPs  using Ni-std

- solve for parameter $\lambda_x$ (IMFP)

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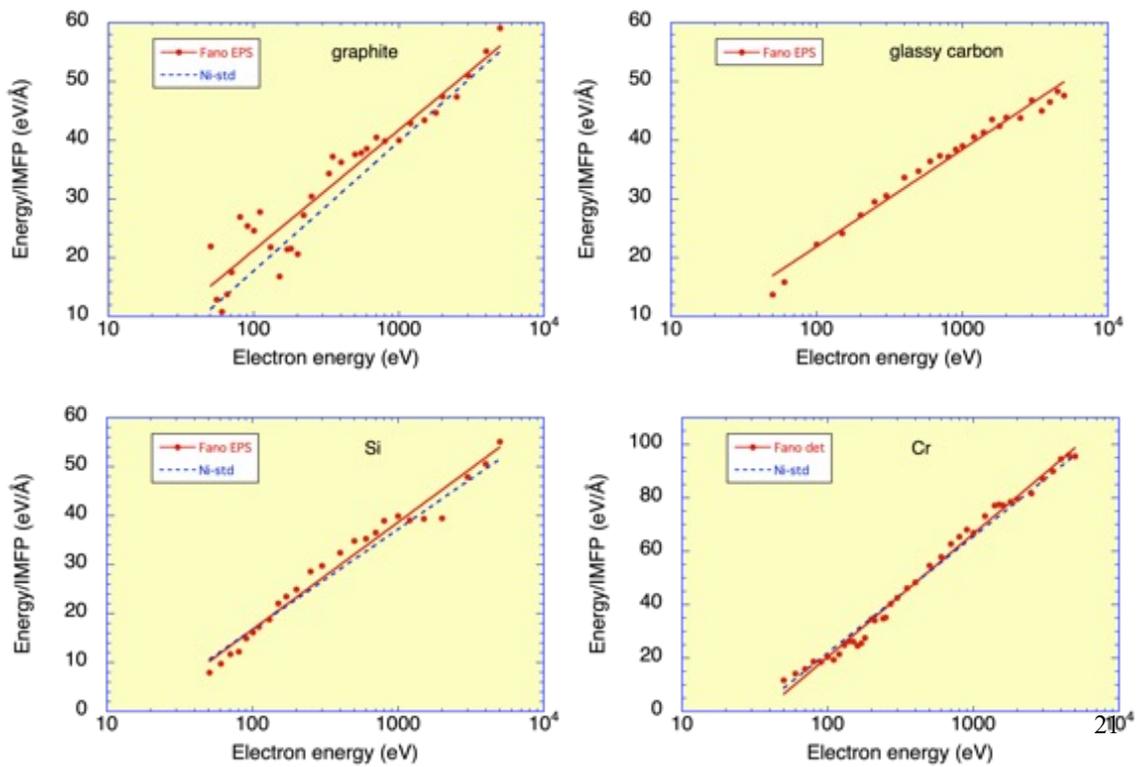


Simple Bethe equation

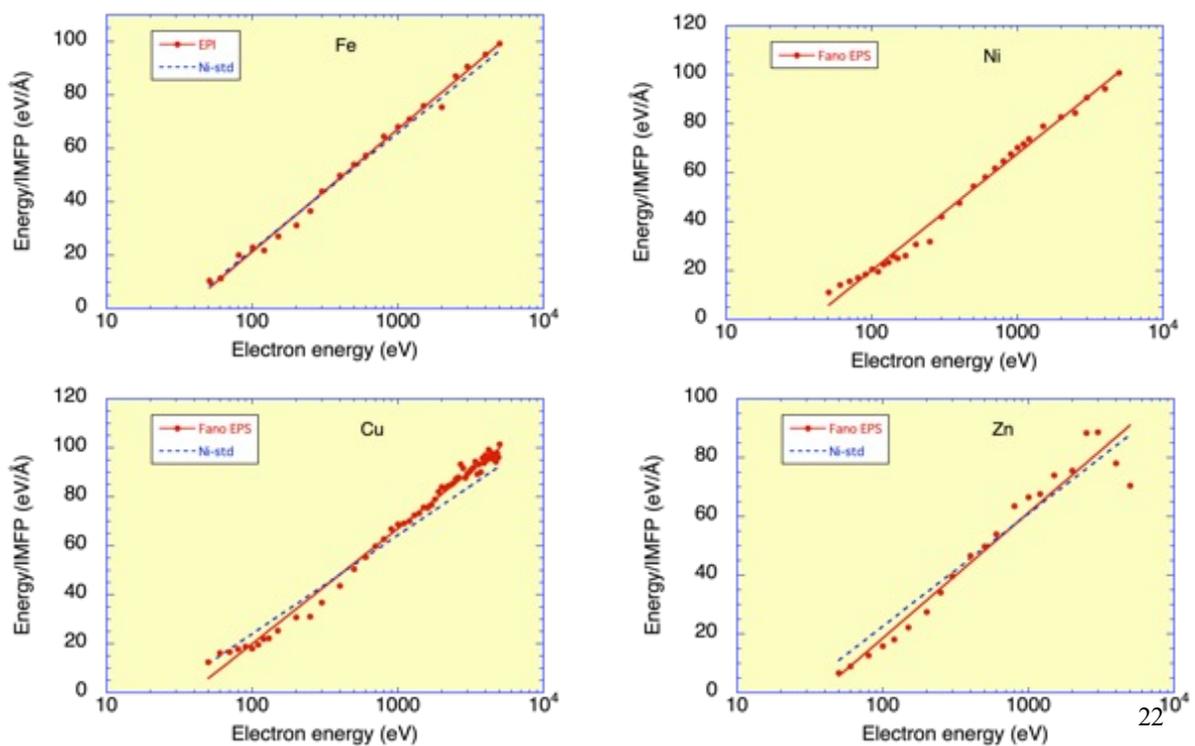$$E/\lambda = b + a\ln(E)$$

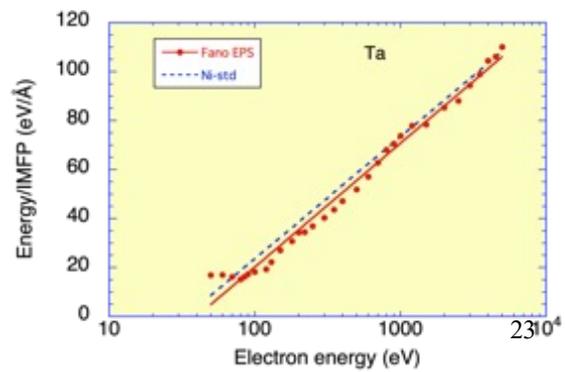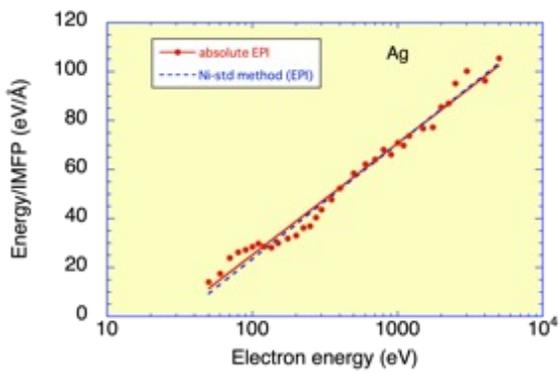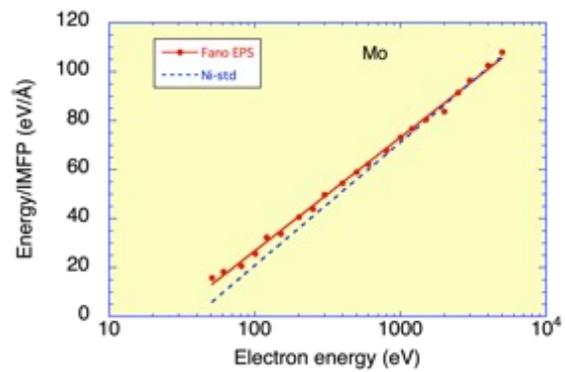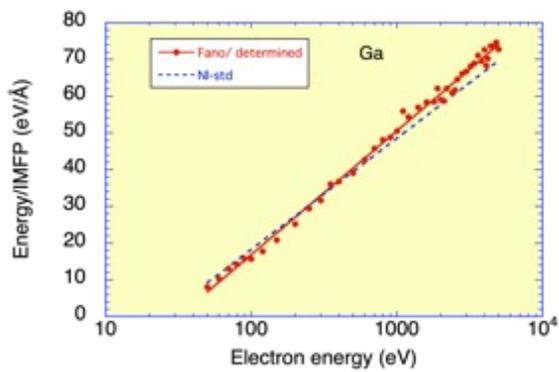: Parameters were determined from curve fits

- dotted line : calculated from  these parameters

20

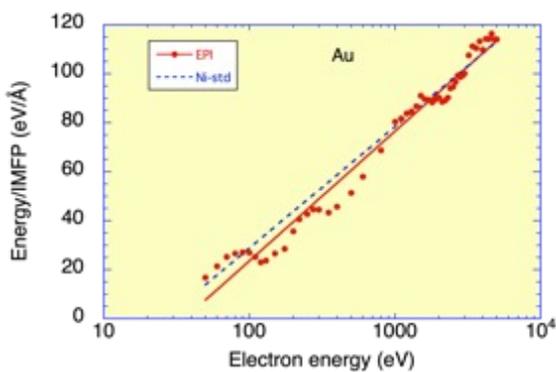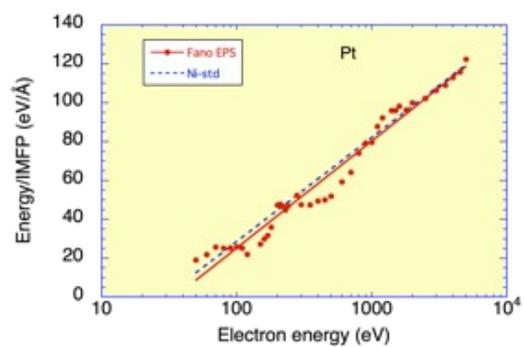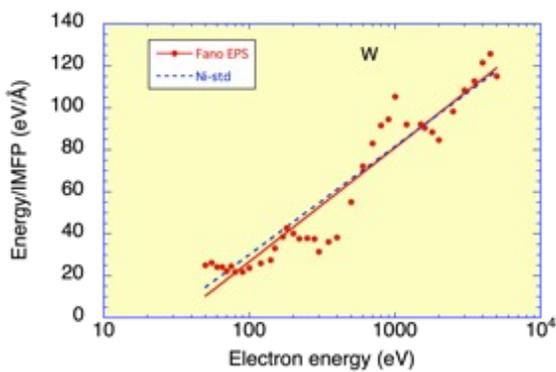# Analysis of IMFPs with Fano Plot(1)

# Analysis of IMFPs with Fano Plot (2)

# Analysis of IMFPs with Fano Plot(3)

# Analysis of IMFPs with Fano Plot (4)

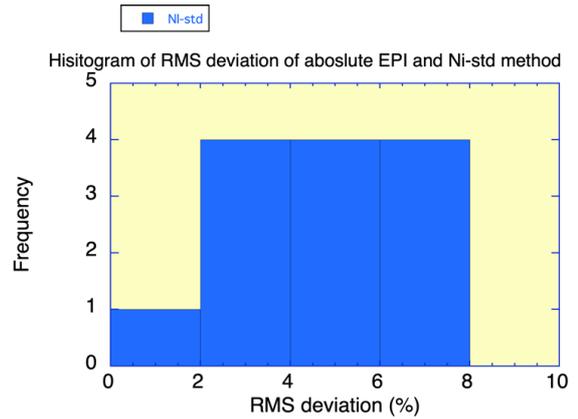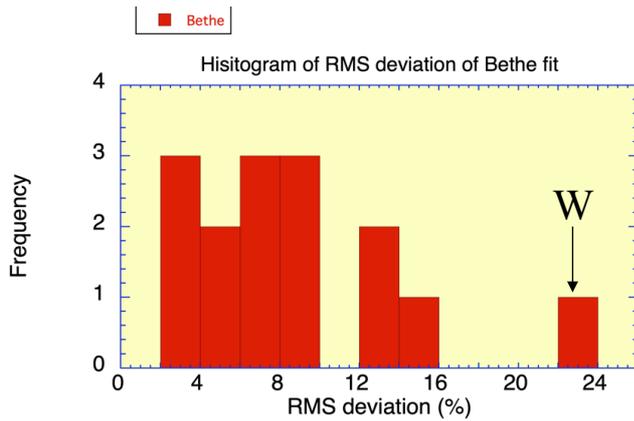# Results of Bethe eq. fits to measured IMFPs in the 100 - 5,000 eV range

- **Average RMS deviation**

Bethe fit:
- present work (from absolute EPI): 8.7 %
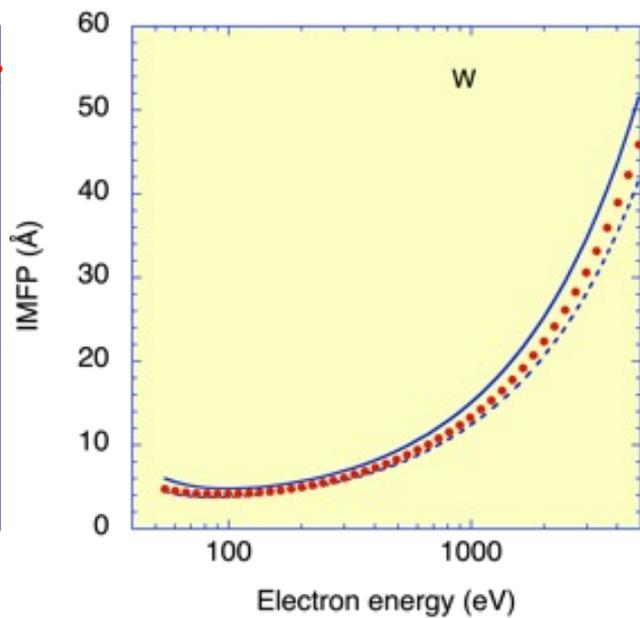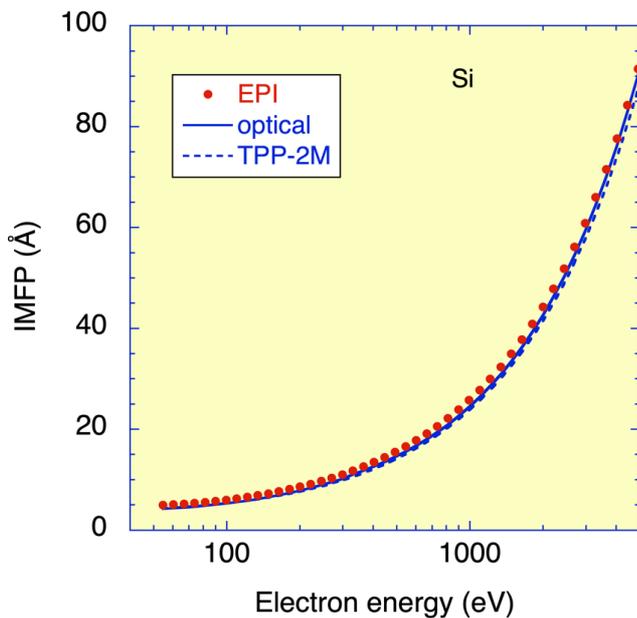- EPI- Ni-ref method : 9.1%

-comparison of Bethe fit results
: absolute EPI (present work)
and  Ni-ref EPI  : 5.0 %

■ Bethe

Hisitogram of RMS deviation of Bethe fit

W



■ NI-std

Hisitogram of RMS deviation of aboslute EPI and Ni-std method



25

# Comparison of resulting IMFPs from the Bethe fit with optical IMFPs , TPP-2M, EPES-Ni-std (Si, W)

Si
- • EPI
- —— optical
- ----- TPP-2M



W



26

IMFP determined from absolute EPI
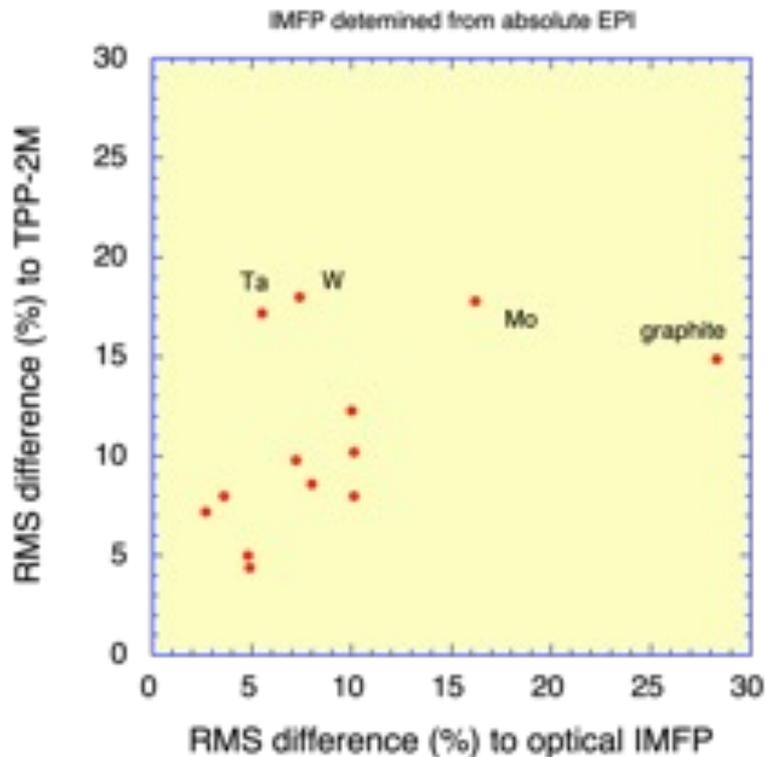


Average RMS(%): 100 - 5000
eV : 9.1 %(optical), 10.8 %(TPP-2M)

average RMS(%): 100 - 5000 eV
: 11.0%(optical), 10.7%(TPP-2M)

27

# Summary

- We have carried out the experimental determinations of IMFPs for 14 elemental solids (Ag, Au,Cr, Cu, Fe, Ga, graphite,(glassy carbon,) Mo, Pt, Si, Ta, W and Zn) in the 50-5000 eV energy range from absolute backscattered elastic-peak intensities taken by a novel CMA with Monte Carlo (MC) calculations and also compared with IMFPs of the elemental solids with the Penn algorithm.

-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%)

28

-The EPES-IMFPs of Ag, Au,Cu, Cr, glassy carbon,Ni, Pt, Si, Ta and W are in excellent agreement (RMS deviations is less than 10%; average:7% ) with those calculated from the Penn algorithm in the 100-5000 eV energy range. The average RMS deviation for 15 elemental solids is about 10%. However, the RMS deviations for Mo and graphite were large;16 and 28 % , respectively.

- Differences between the present EPES-IMFPs and IMFPs from EPES-Ni-ref method are also small (average RMS differences was 5.0 %) in the 100-5000 eV energy range.

-We may conclude that the accuracy of IMFP values for elemental solids calculated from measured ELFs are about 10% in the 100 - 5000 eV energy range.

- Surface-electronic excitation ?