Data Report

Effective Inelastic Mean Free Paths and the elastic scattering factor γ_{el} (I)

- lithium, sodium, potassium, rubidium, aluminum, silicon, copper, silver and gold -

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We report the calculated results of " effective" inelastic mean free paths (EIMFP) and the elastic scattering correctiong factor γ_{el} for Li, Na, K, Rb, Al, Si, Cu, Ag, and Au. The EIMFP is defined as the average straight-distance between two successive inelastic collisions. This quantity is, therefore, expected to be independent on the experimental configuration. The elastic scattering correction factor γ_{el} in solids is defines by the following relation;

$$\lambda_{eff} = \gamma_{el} \times \lambda_{inel}$$

where, λ_{eff} is the EIMFP and λ_{inel} indicates the inelastic mean free path (IMFP).

Calculation method

EIMFP is defined as the average distance between two inelastic collisions. Then, it can be determined from the slope of the straight-distance distribution function (S-DDF) of the electrons in solids. So, we estimated the straight distance distribution (S-DD) by Monte Carlo simulation method. For the estimation, following physical quantities are used.

1) electron inelastic mean free path λ_{inel}

The IMFP λ_{inel} are calculated using the following TPP-2M equation[1]. The parameters β, γ, C, D used in the calculations for Li, Na, K, Al, Si, Cu, Ag, Ag were determined by the curve fit with Eq. (1) to the IMFP values calculated with the Penn algorithm[2]. The details will be published elsewhere [3].

The TPP-2M equation is expressed as

$$\lambda_{inel} = \frac{E}{E_p^2\left[\beta \ln(\gamma E) - C/E + D/E^2\right]} \quad (\text{Å}) \qquad (1)$$

$$\beta = -0.10 + 0.944/\left(E_p^2 + E_g^2\right)^{1/2} + 0.069\,\rho^{0.1} \qquad (2a)$$

$$\gamma = 0.191\,\rho^{-0.5} \qquad (2b)$$

$$C = 1.97 - 0.91\,U \qquad (2c)$$

$$D = 53.4 - 20.8\,U \qquad (2d)$$

The parameters used for the calculations are listed in Table 1.

The total cross section for inelastic scattering is the inverse of the IMFP.

2) electron elastic scattering

The differential cross-section for elastic scattering, $d\sigma^{el}(\theta)/d\theta$, is given by [4],

$$\frac{d\,\sigma^{el}(E)}{d\,\theta} = \left|f(\theta)\right|^2 + \left|g(\theta)\right|^2 \qquad (3)$$

Here, θ denotes scattering angle, and the scattering amplitudes of $f(\theta)$ and $g(\theta)$ are obtained by solving the Dirac equation for Thomas-Fermi-Dirac (TFD) potential. Total cross-section $\sigma^{el}(E)$ is obtained by the integration of Eq.(1), and EMFP (λ_{el}) are obtained by

$$\lambda_{el} = \frac{1}{\left(n\,\sigma^{el}(E)\right)} \qquad (4)$$

where n is atomic density of target materials.

Monte Carlo simulation was carried out using the values of EMFPs and IMFPs as follows. At the first step, path length s which means the distance of the electron traveling to the next collision is estimated by

$$S = -\lambda_m \ln(r) \qquad (5)$$

Here, r is a uniform random number, and λ_m is a mean free path which is given by

$$\frac{1}{\lambda_m} = \frac{1}{\lambda_{inel}} + \frac{1}{\lambda_{el}} \quad (6)$$

Then, in the second step, type of scattering is determined at the next scattering point by the following relations;

$$r_1 < \frac{\sigma^{inel}(E)}{T(E)}, \quad T(E) = \sigma^{el}(E) + \sigma^{inel}(E) \quad (7)$$

When the above relation is satisfied, the inelastic scattering occurs at this point and the MC simulation is stopped. Then we estimate the straight-distance between the original point and the point where inelastic scattering occured.

The calculations were carried out for a series of materials at electron energy between 50 and 2000 eV.

Determination of EIMFP and γ_{el}

The calculated results of S-DD can be expressed by the following equation.

$$I(z) / \int_0^\infty I(z)dz \quad (8)$$

where, z is the straight distance. The EIMFP can be defined as the slope of the S-DDF (Straight-Distance Distribution Function). When the elastic scattering is ignored, the S-DDF F(z) can be expressed as

$$F(z) = \frac{1}{\lambda_{inel}} \exp\left(-\frac{z}{\lambda_{inel}}\right) \quad (9)$$

In analogy,the S-DDF including elastic scattering effect (G(z)) may be given by

$$G(z) = \frac{1}{\gamma_{el}\lambda_{inel}} \exp\left(-\frac{z}{\gamma\lambda_{inel}}\right) \quad (10)$$

where γ_{el} is the elastic scattering factor and $\gamma_{el}\lambda$inel corresponds to the EIMFP.

We have determined γ_{el} value for them from the curve fit with Eq.(10) to the data of S-DD. The calculated results of EIMFP and γ_{el} for Li, Na, K, Rb, Al, Si, Cu, Ag, and Au are shown in Table 2 together with those of IMFP and EMFP. The details of those values are published elsewhere [5].

Table 1. parameters used for IMFP calculation

The parameters β, γ, C, D except for Rb were determined from the curve fitting with Eq.(1) to the data of IMFPs calculated by Penn algorithm, which make use of energy loss function.

***Calculated from Eq.(2a)-(2d).**

Ep are calculated from the following equation.

$$E_p = 28.8\left(\frac{N_v\rho}{Aw}\right)^{1/2} \quad \text{(eV)}$$

where N_v is the number of valence electrons, ρ the density (g/cm^3) and Aw the atomic weight.

Element	β	γ	C	D	Ep (eV)
Li	0.067	0.37	2.43	58.8	7.99
Na	0.131	0.243	5.95	202.6	5.92
K	0.175	0.316	5.31	9.1	4.28
Rb*	0.217	0.154	1.95	53.0	3.86
Al	0.0422	0.0861	0.462	13.9	15.8
Si	0.0329	0.0919	0.543	13.3	16.6
Cu	0.0127	0.0439	0.513	20.6	35.9
Ag	0.02	0.0574	1.69	54.8	29.8
Au	0.0235	0.0424	1.57	55.7	29.9

References

[1] S. Tanuma, C.J. Powell, and D. R. Penn, Surf. Interface Anal., 21, 165 (1994).

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[3] For Si, Cu, Ag and Au : S. Tanuma, C.J. Powell, and D. R. Penn, Surf. Interface Anal.,11, 577 (1988). For Li, Na, K, Rb and Al : S. Tanuma, C.J. Powell, and D. R. Penn (to be published).

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Table 2. Calculated results of γ_{el}, IMFP, EMFP, and EIMFP

	lithium				sodium			
Electron energy(eV)	γ_{el}	IMFP(A)	EMFP(A)	EIMFP(A)	γ_{el}	IMFP(A)	EMFP(A)	EIMFP(A)
50	0.97	4.6	11.1	4.4	0.92	4.9	9.8	4.5
100	0.98	7.0	18.1	6.9	0.92	7.6	11.8	7.0
150	0.97	9.2	25.2	8.9	0.94	9.7	14.3	9.2
200	0.99	11.3	32.3	11.2	0.95	11.8	16.7	11.2
300	0.99	15.3	46.6	15.2	0.95	15.8	21.1	15.0
400	1.00	19.0	60.8	19.1	0.96	19.5	25.1	18.8
500	1.00	22.7	75.1	22.6	0.98	23.2	28.8	22.7
600	0.99	26.3	89.3	26.0	0.96	26.7	32.4	25.7
700	0.98	29.7	103.6	29.2	0.99	30.1	35.9	29.9
800	0.99	33.1	117.8	32.7	1.00	33.5	39.2	33.4
900	0.99	36.5	132.1	36.1	0.99	36.8	42.5	36.3
1000	1.01	39.8	146.4	40.2	1.00	40.1	45.8	40.0
1100	1.01	43.0	160.6	43.3	0.98	43.3	49.0	42.5
1200	1.00	46.3	174.9	46.3	0.98	46.5	52.1	45.4
1300	1.00	49.4	189.1	49.4	0.99	49.6	55.3	49.0
1400	1.00	52.6	203.4	52.8	0.99	52.8	58.4	52.4
1500	1.00	55.7	217.6	55.5	1.00	55.8	61.5	56.1
1600	1.01	58.8	231.9	59.5	0.98	58.9	64.6	57.7
1700	1.00	61.9	246.2	61.7	0.99	61.9	67.6	61.2
1800	0.99	64.9	260.4	64.3	1.00	64.9	70.7	64.9
1900	1.00	68.0	274.7	67.8	0.99	67.9	73.7	67.4
2000	0.99	71.0	289.0	70.4	1.00	70.9	76.7	70.7

	potassium				rubidium			
Electron energy(eV)	γ_{el}	IMFP(A)	EMFP(A)	EIMFP(A)	γ_{el}	IMFP(A)*	EMFP(A)	EIMFP(A)
50	0.96	7.2	9.0	6.9	0.99	7.9	10.4	7.8
100	0.94	9.9	15.1	9.3	0.97	11.6	14.4	11.2
150	0.94	12.8	19.5	12.1	0.94	15.0	17.7	14.2
200	0.94	15.7	22.8	14.7	0.93	18.3	20.4	17.0
300	0.95	21.1	28.1	20.0	0.92	24.4	24.6	22.4
400	0.96	26.3	32.6	25.2	0.93	30.3	27.9	28.1
500	0.96	31.3	36.7	30.0	0.92	35.8	30.8	33.0
600	0.97	36.2	40.5	35.0	0.92	41.2	33.5	38.1
700	0.97	40.9	44.1	39.6	0.93	46.5	36.1	43.1
800	0.97	45.6	47.6	44.3	0.92	51.6	38.5	47.3
900	0.97	50.2	51.0	48.5	0.95	56.7	40.8	54.1
1000	0.97	54.7	54.3	53.1	0.94	61.7	43.0	58.0
1100	0.98	59.1	57.5	58.0	0.94	66.6	45.2	62.5
1200	0.97	63.5	60.7	61.5	0.94	71.4	47.2	67.5
1300	0.98	67.9	63.8	66.5	0.96	76.2	49.3	73.1
1400	0.98	72.2	66.8	71.0	0.96	80.9	51.2	77.7
1500	0.99	76.5	69.8	75.7	0.97	85.6	53.2	82.8
1600	0.99	80.7	72.7	80.2	0.96	90.2	55.1	86.3
1700	0.98	84.9	75.6	83.2	0.96	94.8	56.9	91.1
1800	0.99	89.1	78.5	88.3	0.96	99.3	58.7	95.8
1900	0.98	93.2	81.4	91.3	0.95	103.8	60.5	99.1
2000	0.99	97.3	84.2	96.1	0.96	108.3	62.2	104.0

IMFPs for Li, Na, K were calculated from Eq.(1) and the parameters listed in Table1.
* IMFPs for Rb were calculated from Eq.(1) and Eq.(2a)-(2d).

Table 2. (continue) Calculated results of γ, IMFP, EMFP, and EIMFP

	aluminum				silicon			
Electron energy(eV)	γ_{el}	IMFP(A)	EMFP(A)	EIMFP(A)	γ_{el}	IMFP(A)	EMFP(A)	EIMFP(A)
50	0.89	3.5	4.4	3.1	0.90	4.1	4.9	3.6
100	0.88	4.6	4.8	4.0	0.88	5.3	5.6	4.7
150	0.90	5.7	5.6	5.1	0.90	6.5	6.5	5.9
200	0.91	6.8	6.4	6.2	0.91	7.8	7.4	7.1
300	0.92	8.9	7.9	8.2	0.93	10.1	9.0	9.5
400	0.95	10.8	9.3	10.3	0.95	12.4	10.6	11.7
500	0.95	12.7	10.6	12.1	0.95	14.5	12.1	13.8
600	0.96	14.5	11.8	13.9	0.95	16.6	13.4	15.8
700	0.98	16.3	13.0	15.9	0.97	18.7	14.8	18.1
800	0.97	18.1	14.2	17.5	0.97	20.7	16.1	20.0
900	0.97	19.8	15.3	19.1	0.96	22.6	17.3	21.8
1000	0.98	21.4	16.5	21.0	0.95	24.5	18.6	23.4
1100	0.97	23.1	17.5	22.4	0.98	26.4	19.8	26.0
1200	0.98	24.7	18.6	24.3	0.99	28.3	21.0	27.9
1300	0.97	26.3	19.7	25.5	0.98	30.1	22.1	29.4
1400	0.99	27.9	20.7	27.5	0.97	31.9	23.3	31.0
1500	0.99	29.4	21.8	29.2	0.99	33.7	24.4	33.4
1600	0.99	31.0	22.8	30.8	0.98	35.5	25.5	34.9
1700	0.99	32.5	23.8	32.0	0.98	37.2	26.7	36.5
1800	0.99	34.0	24.8	33.9	0.98	39.0	27.8	38.4
1900	0.99	35.5	25.9	35.1	0.98	40.7	28.9	40.0
2000	0.99	37.0	26.9	36.8	1.00	42.4	30.0	42.4

	copper				silver			
Electron energy(eV)	γ_{el}	IMFP(A)	EMFP(A)	EIMFP(A)	γ_{el}	IMFP(A)	EMFP(A)	EIMFP(A)
50	0.85	4.9	4.3	4.2	**	6.1	1.8	**
100	0.86	4.9	2.9	4.2	0.88	4.8	2.0	4.2
150	-	5.4	2.8	-	-	4.9	2.6	-
200	0.85	6.1	3.0	5.1	0.92	5.4	3.1	4.9
300	0.85	7.5	3.5	6.3	0.90	6.5	3.9	5.9
400	0.86	8.8	4.0	7.6	0.89	7.7	4.5	6.8
500	0.86	10.2	4.4	8.7	0.89	8.8	5.0	7.9
600	0.88	11.4	4.8	10.1	0.90	9.9	5.4	8.9
700	0.89	12.7	5.2	11.3	0.89	11.0	5.9	9.9
800	0.89	13.9	5.6	12.5	0.90	12.1	6.2	10.9
900	0.91	15.2	6.0	13.8	0.90	13.1	6.6	11.8
1000	0.91	16.4	6.3	14.9	0.90	14.2	7.0	12.8
1100	0.92	17.5	6.7	16.1	0.92	15.2	7.3	13.9
1200	0.93	18.7	7.0	17.3	0.92	16.2	7.6	14.9
1300	0.94	19.8	7.3	18.6	0.91	17.2	7.9	15.7
1400	0.94	20.9	7.6	19.6	0.93	18.2	8.2	17.0
1500	0.94	22.1	7.9	20.7	0.92	19.2	8.5	17.7
1600	0.95	23.2	8.2	22.0	0.93	20.2	8.8	18.8
1700	0.95	24.3	8.5	23.1	0.93	21.1	9.1	19.6
1800	0.94	25.3	8.8	23.8	0.92	22.1	9.3	20.4
1900	0.95	26.4	9.1	25.0	0.93	23.0	9.6	21.3
2000	0.95	27.5	9.4	26.0	0.94	23.9	9.9	22.5

IMFPs were calculated from Eq.(1) and the parameters listed in Table1.

** Could not determined because S-DD did not vary exponentially with depth.

- : not calculatednot calculated

Table 2. (continue) Calculated results of γ, IMFP, EMFP, and EIMFP

		gold		
Electron energy(eV)	γ_{el}	IMFP(A)	EMFP(A)	EIMFP(A)
50	**	6.6	1.7	**
100	0.92	4.7	1.7	4.3
150	-	4.7	1.9	-
200	0.94	5.1	2.1	4.8
300	0.93	6.1	2.8	5.7
400	0.92	7.1	3.4	6.6
500	0.90	8.1	3.9	7.3
600	0.90	9.1	4.3	8.2
700	0.90	10.1	4.6	9.1
800	0.89	11.1	4.9	9.9
900	0.89	12.0	5.2	10.7
1000	0.89	12.9	5.4	11.5
1100	0.89	13.8	5.7	12.3
1200	0.90	14.7	5.9	13.2
1300	0.89	15.6	6.1	13.9
1400	0.90	16.5	6.3	14.8
1500	0.89	17.4	6.5	15.4
1600	0.89	18.2	6.7	16.2
1700	0.89	19.1	6.9	17.1
1800	0.90	19.9	7.1	18.0
1900	0.89	20.8	7.3	18.5
2000	0.90	21.6	7.4	19.5

IMFPs were calculated from Eq.(1) and the parameters listed in Table1.

** Could not determined because S-DD did not vary exponentially with depth.

- : not calculatednot calculated