Determinations of IMFPs for 50 - 5000 eV in Copper with Absolute Elastic Scattering Electron Spectroscopy

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We have determined of Inelastic Mean Free Paths (IMFPs) of Copper in the range 50 -5000 eV from the absolute elastic scattering electron intensity measured by Goto's absolute spectrometer together with Monte Carlo method. The resulting IMFPs of copper were smaller than those of IMFPs calculated from the Penn algorithm using energy loss function when the surface excitation correction were ignored. Then, we have estimated surface excitation probabilities for copper in the range 300 - 5000 eV from the intensity ratios of the measured elastic peaks and the calculated intensities from the Monte Carlo method using IMFP values calculated from the Penn algorithm.

1. Introduction

Electron inelastic mean paths (IMFPs), effective attenuation lengths (EALs), and escape depths (EDs) are very important physical quantities for surface analyses by AES and XPS. The IMFP is the most basic parameter. Values of IMFPs have been determined from theoretical calculations[1] because reliable experimental determinations of the IMFP is a rather complicated task. It is very important to compare IMFPs calculated from theory with experimental values in order to check the reliability of the IMFPs.

Elastic peak electron spectroscopy is an efficient tool for experimental determination of IMFPs. This method, usually, requires a reference sample to obtain values of IMFPs and gave different values according to choice of the reference specimen [2]. We have here determined IMFPs of copper using absolute electron elastic scattering spectroscopy. The absolute elastic peak intensities were measured by a novel cylindrical mirror Auger electron analyzer equipped with a Faraday cup[3].

2. Experimental

2.1 Measurement

The energy dependence of the elastically backscattered primary electron current of copper has been measured with a novel cylindrical analyzer (CMA) in the range 1 - 5000 eV [4]. Each elastic peak height was corrected for energy resolution and the EN(E) characteristics and normalized to the primary current (1 μA).

The used copper specimen was a polycrystal, and was polished with alumina paste. Before measurements, the specimen surface was cleaned by Ar^+ sputtering at 600 eV to remove surface contaminations.

The electron transmission efficiency of CMA mesh was estimated from the measurement of the mesh transmission efficiency of laser light, in which the incident angle is 42.3 degree from the surface normal. The resulting values is in good agreement with the efficiency calculated from the size of the mesh at 42.3 degree from the surface normal.

2.2 Calculation

The elastic scattered intensity of electron is calculated by the Monte Carlo method with the following equation.

$$\frac{I}{I_0} = F_t \times f_s \times \int_0^{\infty} \left(\frac{d\eta}{dS}\right) / N_0 \exp\left(-\frac{S}{\lambda}\right) dS \qquad (1)$$

where F_t is the transmission efficiency of the CMA mesh, f_s is a surface excitation correction factor, $d\eta / dS$ is a histogram of the number of electrons versus total path length S of the elastic scattered electrons detected by the CMA, and λ is the electron inelastic mean free path IMFP, and N_0 is the number of input electrons. In the

calculation of $d\eta / dS$, the Thomas-Fermi-Dirac Potential was used for the elastic scattering.

We have calculated elastic electron intensities at 50 eV, 100 - 2000 eV (100 eV step) and 2500 - 5000 eV (500 eV step) with the Monte Carlo method using the above equation. Since we need a very huge number of random numbers in the calculation, its generator plays an important role. We used, then, the Mersenne Twister which is a pseudo-random number generator developed by M. Matsumoto et al.[4]. It is proved that the period is 2^19937-1, and the 623-dimensional equidistribution property is assured. We also used IMFP values calculated from the Penn algorithm using an optical energy loss function for copper [1] in the Monte Carlo calculations of elastic peak intensities. The IMFP parameter values, however, were changed until the calculated intensity was equal to the corresponding measured intensity.

3. Results and Discussion

3.1 Energy dependence of elastic peak intensity

The elastic-scattered electron intensities of Cu from the Monte Carlo method and those absolutely measured by the novel CMA are shown in Fig.1. In the calculations, we ignored the surface excitation correction (f_s=1). From this figure, we can see the calculated intensities are larger than the measured ones by about 30 - 140% in the range 100 - 5000 eV. The reason is believed to be mainly due to the surface excitation effect (SEE). However, the energy dependencies of the calculated and measured elastic peak intensities are similar.

The measured intensity at around 1200 eV in Fig.1 deviates from the smoothed curve line. We do not know the reason.

3.2 Comparison of surface excitation correction

Using the surface plasmon excitation probability P_s, the surface excitation correction (SEC) factor f_s can be described as

$$P_s(\alpha, E) = \frac{\pi}{4v}\frac{1}{\cos(\alpha)} \quad (2)$$

where α_{in} means the electron incident angle to the surface normal, α_{out} means the angle of the detected electrons, and E is the electron energy.

Chen [6] determined a general formula for P_s using a free electron gas model together with the surface energy loss function;

$$f_s = \exp\left(-P_s(\alpha_{in}, E)\right)\exp\left(-P_s(\alpha_{out}, E)\right) \quad (3)$$

Where $v = \sqrt{2E}$.

On the other hand, Oswald gave the following equation for P_s [6].

$$P_s(\alpha, E) = \frac{\frac{\pi}{2a_0 k}}{\cos(\alpha) + \frac{\pi}{2a_0 k}} \quad (4)$$

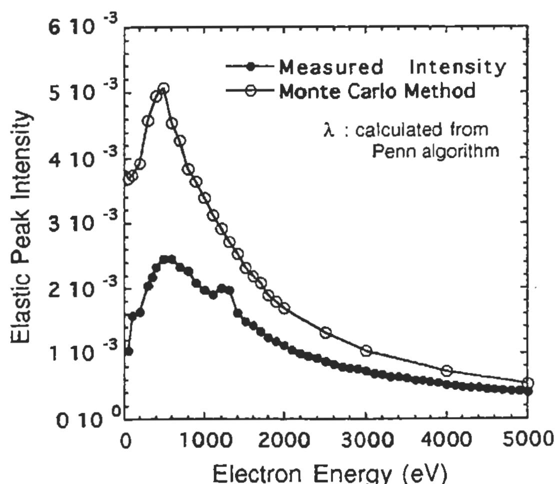

Figure 1. Energy dependence of elastic peak intensities measured by a novel CMA with a Farady cup and those from the Monte Carlo method using IMFPs detemined from the Penn algorithm.

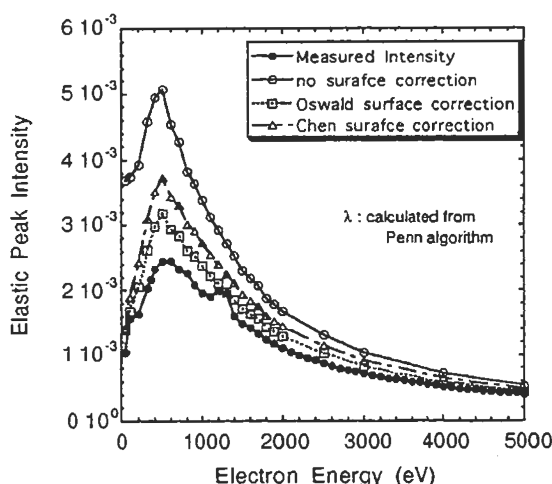

Figure 2. Energy dependence of elastic peak intensities measured by a novel CMA and those from the Monte Carlo method, which were corrected by surface excitation effect using Chen and Oswald equations for P_s.

Where k is the wave number, and a_0 is the Bohr radius. The elastic peak intensities corrected by f_s from equations (3) and (4) are shown in Fig. 2. This figure shows that the measured elastic peak intensities corrected by each surface excitation equation where in better agreement with the calculated intensities than no surface correction was made. However, the difference between the measured intensities and the calculated intensities with the Oswald and Chen corrections is still large. Therefore, the use of the surface excitation correction from equations (3) or (4) is helpful, but the accuracy of these equations might be unreliable.

3.3 IMFPs from Elastic Peak Intensities

The IMFPs of Cu can be determined from equation (1) without a standard specimen because we have measured the absolute value of the elastic peak intensity. The parameter λ in equation (1) was changed until the calculated intensity was equal to the measured values. The resulting IMFPs are shown in Fig. 3. This figure shows that the IMFP values without the SEC are smaller than those from the Penn algorithm by 20 - 50% in the range 500 - 5000 eV. A major factor for the difference between them is believed to be the surface plasmon excitation effect. Corrected IMFPs from Chen or Oswald equation are also shown in Fig. 3. This Figures shows that the resulting IMFPs are still smaller than those from the Penn algorithm. Figure 3 indicates that the SEC could be the most important factor for the determination of IMFPs from measurements of the absolute elastic electron intensity.

As we stated in 3.2, there is still some ambiguity about the accuracy of the SEC. It might be impossible to obtain accurate IMFP value at this time.

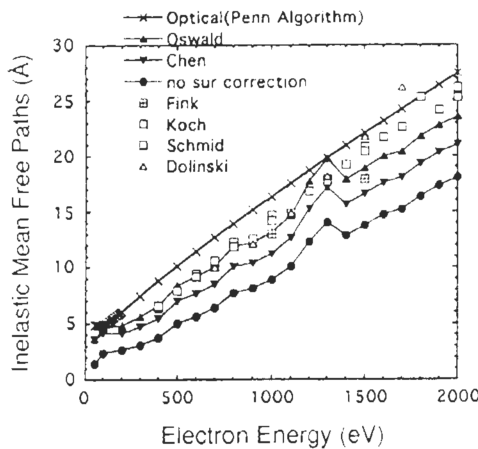

Fig.3 Comparison of IMFPs for Copper in the range 50 - 2000 eV.

X: calculated IMFPs from optical energy loss function using the Penn algorithm. ●: IMFPs determined from elasic peak with equation (1). Oswald and Chen means the surafce correction from Eqs. (3) and (4) ,respectively. The other symbols are the experimental values of IMFPs cited in [8].

3.3 Estimation of Surface Correction Factor

Based on the assumption that the IMFPs determined by the Penn algorithm from the energy loss function and that the measured absolute intensities taken by the novel CMA are correct, we determined the values of the surface excitation correction using the following equation (from equation(1)).

$$f_s^{OBS} = \frac{F_t \int_0^\infty \left(\frac{d\eta}{dS}\right) / N_0 \exp\left(-\frac{S}{\lambda}\right) dS}{\left(\frac{I}{I_0}\right)_{measured}} = \frac{\left(\frac{I}{I_0}\right)_{MC}}{\left(\frac{I}{I_0}\right)_{measured}} \qquad (5)$$

The energy dependence of the surface correction factor f_s for copper is shown in Fig.

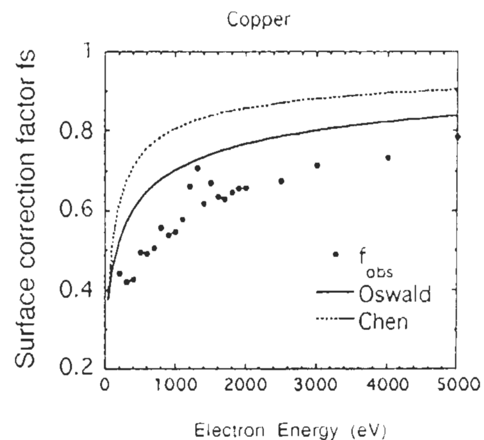

Fig.4 Energy dependence of f_{obs}. Solid squares were obtained from eq.(5). The others were calculated from equations (1),(2), and (3).

4 together with f_s data from Chen and Oswald. The resulting f_{obs} values were smaller than the calculated values by 10 - 30 % in the range 1000 -5000 eV. On the other hand, the difference between the Chen and Oswald values is about 10% in the same energy range. However, the energy dependence of f_{obs} in Fig. 4. resembles that of the Oswald and Chen equations.

The surface excitation probability P_s can be obtained from the following relations.

$$P_s^{total}(E) = -\log(f_s)$$

$$= -\log\left(\left(\frac{I}{I_0}\right)_{MC} / \left(\frac{I}{I_0}\right)_{measured}\right) \quad (6)$$

where $Ps^{total} = Ps^{in} + Ps^{out}$. The P_s values are shown in Fig. 5. If the surface excitation probability for the incident electrons is the same as that of the detected electrons at the same angle to the surface normal, Ps^{total} can be described as

$$P_s^{total}(E) = P_s(E)\left(1 + \frac{1}{\cos(42.3)}\right) \approx 2.35\, P_s(E) \quad ....(7)$$

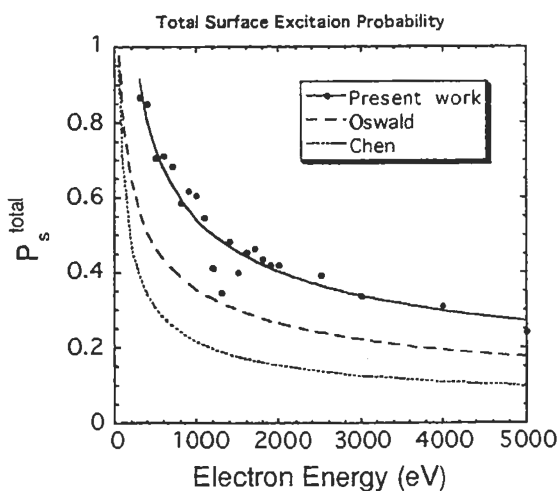

Fig5. Energy dependence of the total surface excitation probability. The solid squares were calculated from equation(6). The otheres (Oswald and Chen) were obatined from equation (3) or (4) and $Ps^{total} = Ps^{in} + Ps^{ou}$.

because the emission angle of the detected electrons in the CMA is 42.3±6°.

The obtained P_s values in Fig.5 can be fitted by the following equation.

$$P_s(\alpha, E) = \frac{1}{\cos(\alpha)}\, a\, E^{-b} \quad (8)$$

where a = 5.33 and b=4.33. The resulting P_s^{total} from equation (8) are shown in Fig.5 as a solid line. These values are larger than those found from the Chen and Oswald equations. However, their energy dependence resembles those of the Chen and Oswald equations. Although the absolute values of the resulting surface excitation probability described by equation (7) might be uncertain due to the surface roughness of the specimen, the effect of the surface crystallinity of the specimen, the transmission efficiency of the CMA mesh etc., its energy dependence must be correct. Therefore, the energy dependence of surface excitation probability can be described by equation (7).

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4. References

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