

Calculations of "Effective " Inelastic Mean Free Paths in Solids

S. Tanuma, S. Ichimura*, and K. Yoshihara**

Japan Energy ARC Co. Ltd., 3-17-35 Niizo-Minami, Toda, Saitama 335, Japan

** Electrotechnical Laboratory, 1-1-4 Umezono, Tukuba, Ibaraki 305, Japan*

*** National Research Institute for Metals, 1-2-1 Sengen, Tukuba, Ibaraki 305, Japan*

(Received April 19, 1996)

We have calculated the effective inelastic mean free paths (EIMFPs) for electrons in some elemental solids; i.e. Li, Na, K, Rb, Al, Si, Cu, Ag, and Au in the range 50 - 2000 eV using Monte Carlo Simulation. In conclusion, the values of EIMFP could be expressed as $\lambda_{\text{EIMFP}} = \lambda_{\text{elastic}} \times y$, where y is a coefficient of the effect of the elastic scattering and λ_{elastic} the inelastic mean free path, in the range 100 - 2000 eV for all calculated elements.

1. Introduction

The electron inelastic mean free paths(IMFPs), attenuation lengths (ALs), and escape depth (ED) are very important physical quantities for surface analyses by Auger and photoelectron spectroscopy. These terms have different definitions; yet many authors are unfortunately unaware of this fact and use these terms interchangeable[1].

In these quantities, IMFP must be the most basic one. There are still some problems to use IMFPs for the quantitative analysis by XPS and AES directly because it ignores the elastic scattering effect completely. On the other hand, AL include the elastic scattering effect where determined experimentally with the thin film method.

.....

.....

2. Calculation

.....

.....

The differential cross-section, for elastic scattering used in the simulation, is given by the following equation [5].

$$\frac{d\sigma_{\text{el}}(E)}{d\Omega} = |f(\theta)|^2 + |g(\theta)|^2 \quad (1)$$

Here, θ denotes the scattering angle, and the scattering amplitudes $f(\theta)$ and $g(\theta)$ are obtained by solving the Dirac equation using the partial wave expansion method[6]. We adopted the analytical expression for the Thomas-Fermi-Dirac (TFD) potential, which

is taken electron screening effects into account, for the calculation.

.....

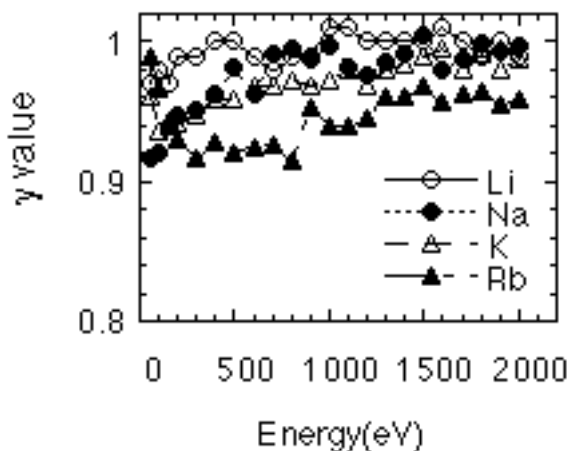


Figure 2. The y values for alkaline metals. These values were obtained from the curve fitting to the normalized intensities calculated by Monte Carlo method with the Eq. (7).

.....

.....

5. References

- [1] C. J. Powell, J. Electron Spectrosc. Relat. Phenom. 47, 197 (1988).
- [2] A. Jablonski, Surf. Sci., 188, 164 (1987)
- [3] D. R. Penn, Phys. Rev. B, 35, 482 (1987).
- [4] S. Tanuma, C.J. Powell, and D. R.Penn, Surf. Interface Anal., 21, 165 (1994).

- [5] S. Ichimura, Surface Science in Japan, 11, 604 (1990).
- [6] N. F. Mott and H. S. W. Massey, The Theory of Atomic Collisions (Oxford Univ. Press, London, 1965).