

tions. This area is expressed as the full width at half maximum of the photoelectron intensity observed as a function of distance from the center of the imaged area. Thus, the effective

sample area is not large. It is often possible to analyze different positions on the same sample when the surface is heterogeneous on a scale larger than two millimeters.

6. How to Use This Handbook

Full utilization of this Handbook can best be accomplished by following these procedures.

A. FOR QUALITATIVE ANALYSIS

The elemental and chemical identification of sample constituents can be performed most readily by combining the information in the standard survey spectra in Section II with the binding energy tables (Tables 1-4) presented in the Appendix.

- (1) First identify all major photoelectron peaks utilizing the line position tables (Tables 1-4, pages 182-187).
- (2) Check to see that the determinations made in step 1 are consistent with the standard survey spectra.
- (3) Identify the Auger electron peaks by the line positions listed in Tables 1-4 in the Appendix (these are different for Mg and Al x-ray sources) and the expanded spectra provided for many of the elements in Section II.
- (4) Review section I.5.A. (p. 12) to account for fine structure such as energy loss lines, shake-up peaks, satellite lines, etc. not identified in Handbook spectra or energy tables.

(5) Identify any remaining small peaks, assuming they are intense photoelectron or Auger lines of minor constituents using Tables 3 and 4.

(6) Chemical state identification can be deduced from high energy resolution ($E_{\text{pass}} \leq 25 \text{ eV}$) spectra of the strongest photoelectron lines and sharpest Auger lines.

i. Review Section I.5.C. (p. 17) to correct binding energies for static charging of insulators. When applicable, charge reference the binding energy scale to the hydrocarbon C1s photoelectron peak ($BE = 284.6 \text{ eV}$).

ii. Use the tabulated experimental data and standard high energy resolution spectra to determine the chemical state from measured shifts in the photoelectron binding energies (cf section I.5.C., p. 18).

iii. For the elements F, Na, Cu, Zn, As, Cd, In, and Te, convert corrected Auger line positions to kinetic energies by subtracting from the photon energy ($Mg = 1253.6$, $Al = 1486.6 \text{ eV}$). Note the location of the points for Auger kinetic energy and photoelectron binding energy on the respective elemental plot. Proximity of experimental points to

those of recorded chemical states should be considered probable identification, if consistent with other elemental findings and with calculated stoichiometry (see below). Note that experimental error in point location is much greater along the Auger parameter grid than normal to the grid lines.

- iv. As suggested in the text (Section I.5.C., p. 20), much can be determined about the chemical state from the magnitude and position of shake-up lines as well as the energy and shape of valence Auger electron lines.

B. FOR QUANTITATIVE ANALYSIS

The atomic sensitivity factors (S_x) presented in Table 5 of the Appendix (p. 188) were calculated according to theoretical photoelectron cross sections, the kinetic energy dependence of the PHI Precision Electron Energy Analyzer and an average value for the dependence of the electron escape depth on kinetic energy. A simplified expression to determine the atomic

concentration (C_x) of any element x is given in equation 8:

$$C_x = \frac{I_x/S_x}{\sum I_i/S_i} \quad (9)$$

where I_x is the relative peak area of photoelectrons from element x . However, it must be pointed out that the method is limited in accuracy by the assumptions made (cf Section I.5.D., p. 21).

The spectrum should be examined with a view to finding information on the depth of the element (i.e., by peak intensity ratios, or the presence or absence of loss lines). Further scans with variable take-off angle, or by erosion of the surface, can be made if this point needs further elucidation.

C. FOR A FINAL CHECK

A concluding effort should be made to ensure that quantitative data and the conclusions on chemical state are consistent. This includes quantitative apportionment of an element among two or more chemical states, where that is indicated.