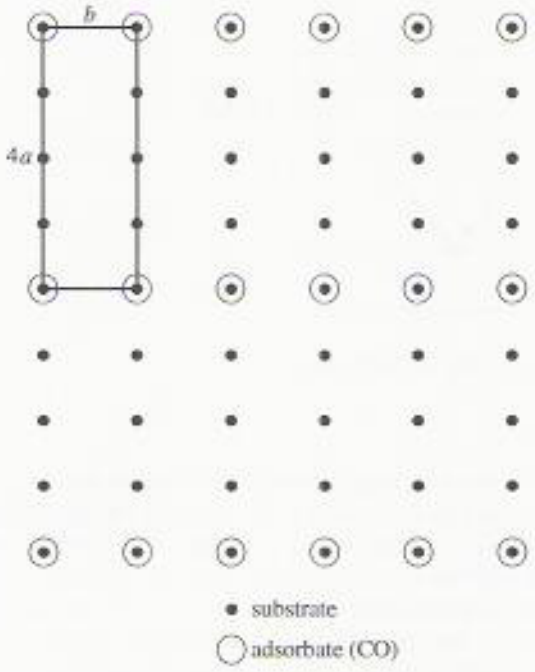

Figure A2 The M(110)(4 × 1)—CO surface structure, with the adsorbate unit mesh marked.

The fractional surface coverage can be defined as

$$\theta = \frac{\text{number of species adsorbed}}{\text{number of substrate atoms in top layer of solid}}$$

where both numbers relate to unit surface area.

The value of θ can be determined by inspection of the adsorbate unit mesh or from the $(m \times n)$ notation:

- As drawn in Figure A2, the adsorbate mesh contains $(6 \times \frac{1}{2} + 4 \times \frac{1}{4}) = 4$ M atoms and $(4 \times \frac{1}{4}) = 1$ CO molecule, so $\theta = \frac{1}{4} = 0.25$.
- Using the notation, $\theta = 1/(m \times n) = \frac{1}{4} = 0.25$.

(*b*) EELS and XPS require clean surfaces. Even at the low operating pressures of these techniques, the surface will be fully covered by contaminants, which must be removed. Methods include the following (any *one* of them):

- heating at low pressure (10^{-11} torr);
- heating in an O_2 atmosphere to oxidize contaminants, with subsequent heating in an H_2 atmosphere to remove any oxide layer;
- argon ion etching to bombard adsorbed contaminants, with annealing to restore surface structure;
- cleaving to expose a clean surface.

(*c*) (*i*) XPS

In XPS, a beam of monochromatic X-ray radiation of given photon energy ($h\nu$) causes the ejection (or ionization) of electrons from core levels of the sample (Figure A3), and the kinetic energies (E_k) of these photoelectrons are analysed. This allows determination of the binding energies (E_B) of the electrons, via the Einstein equation

$$E_k = h\nu - E_B$$

The binding energies of the core electrons in a given element are sufficiently characteristic to be used for qualitative analysis. A table of binding energies of the elements is needed for comparison of E_B values, confirmation of element identification requiring the observation of several possible E_B values. Hence, XPS can provide information both on the composition of a surface, and on the nature of any adsorbed species. Small shifts in expected E_B values may indicate oxidation state values or electron transfer between surface and adsorbate atoms.