approximated (in the model assumed) by

$$\lim_{\Delta E \to 0} (\Delta E)^{-1} \sum_{\substack{\text{states } j \\ \text{in} \\ \Delta E}} \left| C^t_{\ell,m} (j,\underset{\sim}{k}) \right|^2 \times \text{constant}$$

$$= \sum_{\substack{\text{Sheets } j \\ \text{of} \\ \text{Fermi} \\ \text{Surf.}}} \iint \frac{dS_j}{\left|\underset{\sim}{\nabla}_{\underset{\sim}{k}} E_j(\underset{\sim}{k})\right|} \left|C^t_{\ell,m}(j,\underset{\sim}{k})\right|^2 \times \text{constant},$$

for a single polarization and direction of the emitted x-ray. In this expression,

ℓ = 1 for K-emission (metal or non-metal)

2 for L-emission (metal)

1 for M-emission (metal),

$\underline{m}$ is determined by the x-ray polarization (assumed to be circular or parallel to the z axis), and the expansion coefficients $C^t_{\ell m}$ are those for the APW sphere t around the atom in which the transition occurs. For unpolarized x-rays averaged over all angles of emission, the expression becomes proportional to the "partial density of states,"

$$Z^t_\ell (E) = \sum_{\text{Sheets}} \iint \frac{dS_j}{\left|\underset{\sim}{\nabla}_{\underset{\sim}{k}} E_j(\underset{\sim}{k})\right|} \sum_m \left|C^t_{\ell,m} (j,\underset{\sim}{k})\right|^2,$$

which is just the expression for density of states except that

the contribution of each state is weighted by the ℓ-component of its charge in the sphere t of interest [4]. This information is readily available from a self-consistent APW calculation.

The experimental data are reproduced in Fig. 8 and 9. In Fig. 10 is shown the decomposition of the Ti-$L_{II,III}$ emission from TiC, based on the assumption that the two components have the same shape and are separated in energy by the atomic Ti-L_{II}, Ti-L_{III} splitting. The experimental spectra are compared to the computed spectra (arbitrary units for both, no broadening included in the computed curves) in Fig. 11-13 for TiC and in Fig. 14-16 for NbC. In all cases, the calculated Fermi energy has been made coincident with the experimentally determined Fermi energy. For TiC, the curves are also shown with a relative shift of 0.6 eV from this position (dashed curves in Fig. 11 and 13, dot-dash in Fig. 12) which gives even better agreement. The shift to the dashed curve for Nb-$M_{IV,V}$ is to correct for a calibration error in Holliday's data, which was reported by Ramqvist, et. al. [25]. The agreement in all curves is seen to be excellent, if allowance is made for the broadening in the experimental data, which is not included in the theoretical curves.