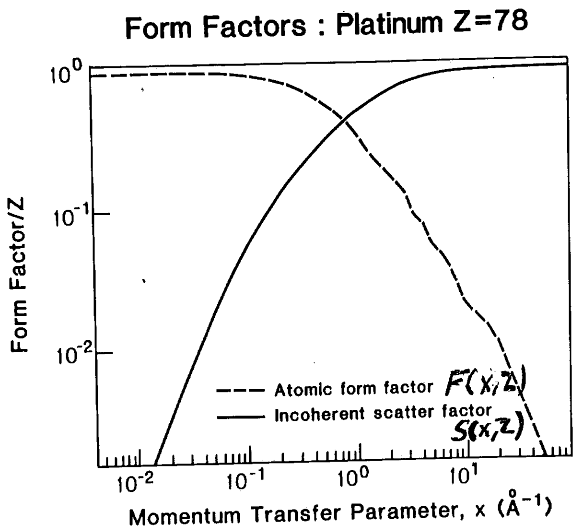

FIGURE 11. Normalized atomic form factors and incoherent scatter functions as a function of momentum transfer parameter x for platinum. Plotted data is from the ENDF/B magnetic tape library (Reference 24).

3. *Sampling from the Incoherent Scattering Differential Cross Section*

Incoherent scattering, often identified with the Compton effect, is an inelastic collision between an atom and an x-ray photon in which the orbital electrons retain part of the photon energy, altering both the energy and flight path of the incident photon. In the energy range of interest, the retained energy is sufficient to ionize the target atom. In the case where the target is a free electron at rest, the effect is properly described as Compton scatter.

As in the free-electron case, we assume that the scattered photon energy E′, (m_oc^2 units) and scattering angle θ are related by

$$E'(\theta) \doteq \frac{E}{1 + E(1 - \cos\theta)} \tag{52}$$

The differential cross section (b/atom-Sr) in the form factor approximation is

$$\frac{d\sigma_{inc}}{d\Omega}(E, \theta, Z) = S(x, Z) \cdot \frac{d\sigma_{kn}}{d\Omega}(E, \theta) \tag{53}$$

where the electronic Klein-Nishina differential cross section is

$$\frac{d\sigma_{kn}}{d\Omega}(E, \theta) = \frac{1}{2} r_e^2 \left(\frac{E'}{E}\right)^2 \left[\frac{E}{E'} + \frac{E'}{E} + \left(\frac{1}{E'} - \frac{1}{E}\right)\left(\frac{1}{E'} - \frac{1}{E} - 2\right)\right] \quad (54)$$

S(x,Z) is the incoherent scatter function and represents the probability that the atom is raised to an excited or ionized state as a result of accepting a recoil momentum 2hx. The momentum transfer parameter is given by

$$x = \frac{m_o c}{2h} [E^2 + E'(\theta)^2 - 2E \cdot E'(\theta) \cos\theta]^{1/2} \quad (55)$$

where m_o, c, and h denote electron rest mass, velocity of light, and Planck's constant, respectively.

As Figure 11 illustrates, S(x,Z) is small for $\theta \simeq 0$ (small x) and approaches Z for large scattering angles. Thus, the effect of electron binding on the KN distribution is to inhibit forward scatter. Since binding corrections are important only for small momentum transfers, the approximation $E \simeq E'(\theta)$ is often made for the purpose of computing x. This allows use of the simple expression (Equation 50) for both coherent and incoherent scattering. The errors introduced into $d\sigma_{inc}$ by this approximation do not exceed 1 to 2%.[19]

A widely used procedure for randomly choosing scattered photon trajectories from Equation 53 is the Kahn two-track rejection technique.[32] Essentially, the procedure is an application of the Butcher composition theorem. First, a change of variables is effected:

$$\lambda = E^{-1}$$

$$\lambda' = E'(\theta)^{-1}$$

$$t = \frac{\lambda'}{\lambda}$$

and

$$2\pi\lambda dt = d\Omega$$

where the last equation follows from Equation 52. Then

$$\begin{aligned} P(t|\lambda) &= \frac{1}{\sigma_{inc}} \frac{d\sigma_{inc}(t, \lambda)}{d\Omega} \frac{d\Omega}{dt} \\ &= \frac{\pi r_e^2}{\sigma_{inc}} \left(\frac{1}{t^2}\right) \left[\frac{1}{t} + t - 1 + (1 - \lambda t + \lambda)^2\right] S(x, Z) \end{aligned} \quad (56)$$

Then define functions $g_1(t)$ and $g_2(t)$, which are PDF normalized over the range of t,[1, 1 + 2/λ], and functions $h_1(t)$ and $h_2(t)$, which take on values confined to the unit interval

$$g_1(t) = \frac{\lambda}{2} \qquad h_1(t) = 4\left(\frac{1}{t} - \frac{1}{t^2}\right) \frac{S(x(t), Z)}{Z}$$

$$g_2(t) = \frac{(\lambda + 2)}{2t^2} \quad h_2(t) = \frac{1}{2}\left[\frac{1}{t} + (1 + \lambda - \lambda t)^2\right] \frac{S(x(t), Z)}{Z} \quad (57)$$

where

$$x(t) = kE \cdot \sqrt{\lambda(t - 1)}$$

Finally,

$$P(t|\lambda) = \frac{\pi r_e^2 Z}{\sigma_{inc}} \left[\frac{1}{2\lambda} g_1(t)\, h_1(t) + \frac{4}{(\lambda + 2)} g_2(t)\, h_2(t) \right] \tag{58}$$

Applying Equation 25, a sample t* is generated by first selecting the "track", i.e., Term 1 or Term 2, obtaining t* by analytical inversion of g_1 or g_2 and applying the decision criterion h_1 and h_2.

Given uniformly distributed random variates r_1^*, r_2^*, $r_3^* \in (0,1)$. Choose track:

$$\begin{aligned} &\text{Track 1} \quad \text{if} \quad r_1^* \leq \frac{\lambda + 2}{9\lambda + 2} \\ &\text{Track 2} \quad \text{if not} \end{aligned} \tag{59}$$

Obtain sample t*:

$$\underline{\text{Track 1}} \quad t^* = \frac{2r_2^*}{\lambda} + 1$$

$$\underline{\text{Track 2}} \quad t^* = \frac{\lambda + 2}{\lambda + 2(1 - r_2^*)}$$

Apply rejection criterion: Accept t* if

$$\begin{aligned} &\text{Accept } t^* \quad \text{if} \\ &\underline{\text{Track 1}} \quad r_3^* \leq h_1(t^*) \\ &\underline{\text{Track 2}} \quad r_3^* \leq h_2(t^*) \end{aligned}$$

If not, repeat entire process.

Given the accepted sample t*, other variables of interest can be easily calculated:

$$\begin{aligned} E'^* &= 1/\lambda t^* \\ w^* &= 1 - \lambda(t^* - 1) \end{aligned} \tag{60}$$

Figure 14 compares the sampled (100,000 samples) and analytically calculated $\Delta\sigma_{inc}/\Delta\Omega$ for 50 and 300 keV photons in platinum. The sampling efficiency ranged from 50% at 100 keV to 63% at 660 keV. At higher energies, efficiency tends to decrease reaching 33% at 10 MeV.

4. Characteristic X-Ray from Photoelectric Absorption

In the photoelectric effect (PE), the incident photon interacts with the tightly bound K, L, or M shell orbital electrons of the target atom. The net result is disappearance of the photon and ejection of the target electron from the atom which carries away the photon energy minus its binding energy. The resultant inner-shell vacancy, when filled by an outer shell electron, gives rise to characteristic x-rays or auger electrons.

Sampling of Eq. 58

$$P(t,\lambda) = \frac{\pi r_e^2 Z}{\nabla_{inc}} \left[\frac{1}{2\lambda} g_1(t) h_1(t) + \frac{4}{(\lambda+2)} g_2(t) h_2(t) \right].$$

Klein-Nishina differential cross section is split into to regimes (tracks).

Must sample to determine track.

$$\text{Total}: \quad \frac{1}{2\lambda} + \frac{4}{(\lambda+2)} = \left(\frac{1}{2\lambda}\right)\left(\frac{9\lambda+2}{\lambda+2}\right)$$

$$\text{Choice of first track}: \quad \frac{\frac{1}{2\lambda}}{\left(\frac{1}{2\lambda}\right)\left(\frac{9\lambda+2}{\lambda+2}\right)} = \frac{\lambda+2}{9\lambda+2}$$

generate random number r_1^*

if $r_1^* \leq \frac{\lambda+2}{9\lambda+2}$ choose track 1

if not choose track 2

Now to sample the functions $g_1(t)$ or $g_2(t)$ for each track. These functions can be inverted analytically. Must generate the cdf for each track on the interval $t: [1, 1+\frac{2}{\lambda}]$

We will following the Generalized Rejection Sampling procedure.

Track 1: $g_1(t) = \frac{\lambda}{2}$

$$r_2^* = G_1(t^*) = \frac{\int_1^{t^*} g_1(t)\,dt}{\int_1^{1+2/\lambda} g_1(t)\,dt} = \frac{\int_1^{t^*} \frac{\lambda}{2}\,dt}{\int_1^{1+2/\lambda} \frac{\lambda}{2}\,dt} = \frac{\frac{\lambda}{2}(t^*-1)}{1}$$

$$\therefore \quad t^* = \frac{2r_2^*}{\lambda} + 1$$

Track 2: $g_2(t) = \frac{\lambda+2}{2t^2}$

$$r_2^* = G_2(t^*) = \frac{\int_1^{t^*} g_2(t)\,dt}{\int_1^{1+2/\lambda} g_2(t)\,dt} = \frac{\int_1^{t^*} \frac{\lambda+2}{2t^2}\,dt}{\int_1^{1+2/\lambda} \frac{\lambda+2}{2t^2}\,dt} = \frac{\lambda+2}{2}\left(1-\frac{1}{t^*}\right)$$

$$\therefore \quad t^* = \frac{\lambda+2}{\lambda+2(1-r_2^*)}$$

Now to apply rejection criterion

Accept t^* if

Track 1 $\quad r_3^* \leq h_1(t^*)$

Track 2 $\quad r_3^* \leq h_2(t^*)$

A total of three random numbers are required to sample the Klein-Nishina differential cross section