φ is the angle of scattering ($= 2\theta$ if θ is the Bragg angle);

$2\pi\,\mathrm{d}(\cos\varphi)$ is the solid angle between cones with angles φ and $\varphi + \mathrm{d}\varphi$;

$f(q, Z)$ is the atomic scattering factor as defined by Cromer & Waber (1974);

q is $[\sin(\varphi/2)/\lambda]$, the momentum transfer parameter. Here λ is expressed in ångströms.

Reliable tables of $f(q, Z)$ exist and have been reviewed recently by Kane, Kissel, Pratt & Roy (1986). The most recent schematic tabulations of $f(q, Z)$ are those of Hubbell & Øverbø (1979) and Schaupp *et al.* (1983). The data used in these tables have been derived from the tabulation for $q = 0.02$ to 10^9 Å^{-1}, for all Z's from 1 to 100 by Hubbell & Øverbø (1979) based on the exact formula of Pirenne (1946) for H, and relativistic calculations by Doyle & Turner (1968), Cromer & Waber (1974), Øverbø (1977, 1978), and high-q extensions using the Bethe–Levinger expression in Levinger (1952).

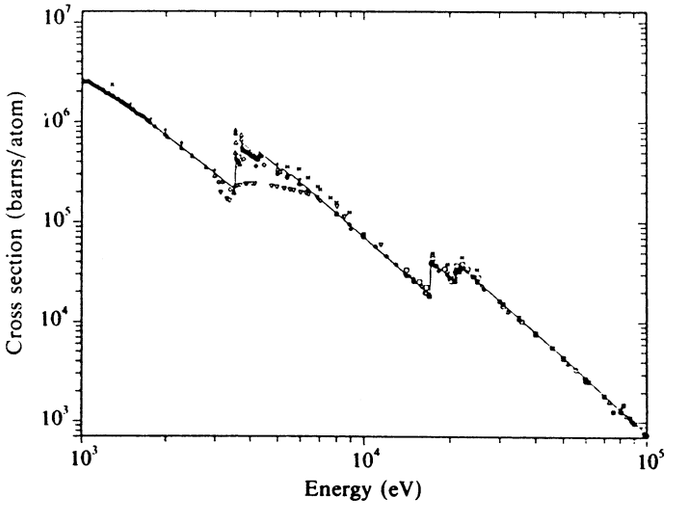

Fig. 4.2.4.3. The total cross section for uranium ($Z = 92$). The theoretical values (solid line) are partially obscured by the high density of available measurements. Deviations of the measured values from the theoretical predictions are mostly of the order of 5%, although a few data sets deviate by more than 30%.

As mentioned in Creagh & Hubbell (1987), the atoms in highly ordered single crystals do not scatter as though they are isolated atoms. Rather, cooperative effects become important. In this case, the Rayleigh scattering cross section must be replaced by two cross sections:

the Laue–Bragg cross section σ_{LB},

and the thermal diffuse scattering cross section σ_{TD}.

That is, σ_R is replaced by $\sigma_{\mathrm{LB}} + \sigma_{\mathrm{TD}}$.

These effects are discussed elsewhere (Subsection 4.2.3.2). Briefly,

$$\sigma_{\mathrm{LB}} = (r_e^2\lambda^2/2NV_c)\sum_H [C_p m d|F|^2 \exp(-2M)]_H. \qquad (4.2.4.7)$$

In equation (4.2.4.7), which is due to De Marco & Suortti (1971),

$C_p = \frac{1}{2}(1 + \cos^2\varphi)$;

d_H is the spacing of the (hkl) planes in the crystal;

m_H is the multiplicity of the hkl Bragg reflection;

F_H is the geometrical structure factor for the crystal structure that contains N atoms in a cell of volume V_c;

$\exp(-2M)_H$ is the Debye-Waller temperature factor.

It is assumed that the total thermal diffuse scattering is equal to the scattering lost from Laue–Bragg scattering because of thermal vibrations.

$$\sigma_{\mathrm{TD}} = (r_e^2\lambda^2/2NV_c)\sum_H \{C_p m d|F|^2[1 - \exp(-2M)]\}_H. \quad (4.2.4.8)$$

H^{1} 20↑ 36↑																	He^{2} 16↑ 2↓
Li^{3} 7↑ 12	Be^{4} 13 17↓											B^{5} 1 *	C^{6} 5↓ 6	N^{7} 6↑ 5	O^{8} 9 6↓	F^{9} 6 3	Ne^{10} 3↓ 5
Na^{11} 11 *	Mg^{12} 4↓ 5											Al^{13} 4 7	Si^{14} 8↓ 2↓	P^{15} 7↓ *	S^{16} 4↓ 3	Cl^{17} 5↑ 2	Ar^{18} 5 14↑
K^{19} 4 *	Ca^{20} 7↓ 12↓	Sc^{21} 6 8↑	Ti^{22} 3 8↑	V^{23} 4↓ 5	Cr^{24} 4 14	Mn^{25} 5↓ *	Fe^{26} 3↓ 29↑	Co^{27} 5↓ 5	Ni^{28} 5 6	Cu^{29} 5 27	Zn^{30} 5↑ 6↑	Ga^{31} 17↑ *	Ge^{32} 3↓ 12	As^{33} 9 *	Se^{34} 7↑ 8↑	Br^{35} 6↑ 4↓	Kr^{36} 2 9↑
Rb^{37} * *	Sr^{38} 5 *	Y^{39} 2↑ 3	Zr^{40} 3↑ 3	Nb^{41} 3 3	Mo^{42} 5↑ 9↑	Tc^{43} * *	Ru^{44} * *	Rh^{45} 4 25	Pd^{46} 3↑ 6↑	Ag^{47} 5↑ 10↑	Cd^{48} 4↑ 13	In^{49} 7↑ 22	Sn^{50} 5↑ 7↑	Sb^{51} 6↑ 42	Te^{52} 9↑ 17↑	I^{53} 5↑ 6↓	Xe^{54} 3 10
Cs^{55} * *	Ba^{56} 4↓ 12↑	La^{57} 7↓ 23↓	Hf^{72} 3 10	Ta^{73} 4 9↓	W^{74} 5 8	Re^{75} * 21↑	Os^{76} * *	Ir^{77} 3 *	Pt^{78} 5↑ 14↓	Au^{79} 4↓ 11↑	Hg^{80} 9 2↑	Tl^{81} 3 *	Pb^{82} 4↑ 6↑	Bi^{83} 7↑ 8↑	Po^{84} * *	At^{85} * *	Rn^{86} * *
Fr^{87} * *	Ra^{88} * *	Ac^{89} * *															
			Ce^{58} 4↑ 3↑	Pr^{59} 2 5	Nd^{60} 3 7↑	Pn^{61} * *	Sm^{62} 4↑ 5↑	Eu^{63} * *	Gd^{64} 3↑ 8↑	Tb^{65} 2 *	Dy^{66} 2 3	Ho^{67} 3 10↑	Er^{68} 3 3	Tm^{69} 2 *	Yb^{70} 3 24↑	Lu^{71} * 80
			Th^{90} 4↓ 11↑	Pa^{91} * *	U^{92} 6 25↑	Np^{93}	Pu^{94}	Am^{95}	Cm^{96}	Bk^{97}	Cf^{98}	Es^{99}	Fn^{100}	Md^{101}	No^{102}	Lr^{103}	

Fig. 4.2.4.4. Comparison between this tabulation and experimental data contained in Saloman & Hubbell (1986). The upper set corresponds to the average percent deviation between the experimental data and this tabulation for the energy range 10 to 100 keV. The lower set corresponds to the energy range 1 to 10 keV. For explanation of symbols see text.

references