of the experiments cited here, however, has claims to high accuracy.

In Table 4.2.6.5, a comparison is made of measurements of $f''(\omega, 0)$ derived from the results of the IUCr X-ray Attenuation Project (Creagh & Hubbell, 1987, 1990) with a number of theoretical predictions. The measurements were made on carbon, silicon and copper specimens at the characteristic wavelengths Cu $K\alpha_1$, Mo $K\alpha_1$ and Ag $K\alpha_1$. The principal conclusion that can be drawn from perusal of Table 4.2.6.5 is that only minor, non-systematic differences exist between the predictions of the several relativistic approaches and the experimental results. In contrast, the non-relativistic theory fails for higher values of atomic number.

4.2.6.3.3.2. *Measurements in the vicinity of an absorption edge*

The advent of the synchrotron-radiation source as a routine experimental tool and the deep interest that many crystallographers have in both XAFS and the anomalous-scattering determinations of crystal structures have stimulated considerable interest in the determination of the dispersion corrections in the neighbourhood of absorption edges. In this region, the interaction of the ejected photoelectron with electrons belonging to neighbouring atoms causes the modulations that are referred to as XAFS. Both $f''(\omega, 0)$ (which is directly proportional to the X-ray scattering cross section) and $f'(\omega, 0)$ [which is linked to $f''(\omega, 0)$ through the Kramers–Kronig integral] exhibit these modulations. It is at this point that one must realize that the theoretical tabulations are for the interactions of photons with *isolated* atoms. At best, a comparison of theory and experiment can show that they follow the same trend.

Measurements have been made in the neighbourhood of the absorption edges of a variety of atoms using the 'direct' techniques interferometry, Kramers–Kronig, refraction of a prism and critical-angle techniques, and by the 'indirect' refinement techniques. In Table 4.2.6.6, a comparison is made of experimental values taken at or near the absorption edges of copper, nickel and niobium with theoretical predictions. These have not been adjusted for any energy window that might be thought to exist in any particular experimental configuration. The theoretical values for niobium have been calculated at the energy at which the experimentalists claimed the experiment was conducted.

Despite the considerable experimental difficulties and the wide variety of experimental apparatus, there appears to be close agreement between the experimental data for each type of atom. There appears to be, however, for both copper and nickel, a large discrepancy between the theoretical values and the experimental values. It must be remembered that the experimental values are averages of the value of $f'(\omega, 0)$, the average being taken over the range of photon energies that pass through the device when it is set to a particular energy value. Furthermore, the exact position of the wavelength chosen may be in doubt in absolute terms, especially when synchrotron-radiation sources are used. Therefore, to be able to make a more realistic comparison between theory and experiment, the theoretical data gained using the relativistic multipole approach (this work) were averaged over a rectangular energy window of 5 eV width in the region containing the absorption edge. The rectangular shape arises because of the shape of the reflectivity curve and 5 eV was chosen as a result of (i) analysis of the characteristics of the interferometers used by Bonse *et al*. and Hart *et al*., and (ii) a statement concerning the experimental bandpass of the interferometer used by Bonse & Henning (1986). It must also be borne in mind that mechanical vibrations and thermal fluctuations can broaden the energy window and that 5 eV is not an overestimate of the width of this window. Note that for elements with atomic numbers less than 40 the experimental width is greater than the line width.

For the Bonse & Henning (1986) data, two values are listed for each experiment. Their experiment demonstrates the effect the state of polarization of the incoming photon has on the value of $f'(\omega, 0)$. Similar X-ray dichroism has been shown for sodium bromate by Templeton & Templeton (1985) and Chapuis *et al*. (1985). The theoretical values are for averaged polarization in

Table 4.2.6.4. *Comparison of measurements of the real part of the dispersion correction for LiF, Si, Al and Ge for characteristic wavelengths Ag $K\alpha_1$, Mo $K\alpha_1$ and Cu $K\alpha_1$ with theoretical predictions; the experimental accuracy claimed for the experiments is shown thus: (10) = 10% error*

Sample	Reference	$f'(\omega, 0)$		
		Cu $K\alpha_1$	Mo $K\alpha_1$	Ag $K\alpha_1$
LiF	Theory			
	This work	0.075	0.017	0.010
	Cromer & Liberman (1981)	0.068	0.014	0.006
	Wagenfield (1975)	0.080	0.023	0.015
	Experiment			
	Creagh (1984)	0.085 (5)	0.020 (10)	0.014 (10)
	Deutsch & Hart (1984*b*)	–	0.0217 (1)	0.0133 (1)
Si	Theory			
	This work	0.254	0.817	0.052
	Cromer & Liberman (1981)	0.242	0.071	0.042
	Wagenfeld (1975)	0.282	0.101	0.071
	Experiment			
	Cusatis & Hart (1975)	–	0.0863 (2)	0.0568 (2)
	Price *et al*. (1978)	–	0.085 (7)	0.047 (7)
	Gerward *et al*. (1979)	0.244 (7)	0.099 (7)	0.070 (7)
	Creagh (1984)	0.236 (5)	0.091 (5)	0.060 (5)
	Deutsch & Hart (1984*b*)	–	0.0847 (1)	0.0537 (1)
Al	Theory			
	This work	0.213	0.0645	0.041
	Cromer & Liberman (1981)	0.203	0.0486	0.020
	Wagenfeld (1975)	0.235	0.076	0.553
	Experiment			
	Creagh (1985)	–	0.065 (20)	0.044 (20)
	Takama *et al*. (1982)	0.20 (5)	0.07 (5)	0.035 (10)
Ge	Theory			
	This work	−1.089	0.155	0.302
	Cromer & Liberman (1981)	−1.167	0.062	0.197
	Wagenfeld (1975)	−1.80	−0.08	0.14
	Experiment			
	Gerward *et al*. (1979)	−1.04	0.30	0.43
	Grimvall & Persson (1969)	−1.79	0.08	0.27

references