11.7—21   EXPERIMENTAL EVIDENCE OF THE "INVERSE ABSORP-
TION ASYMMETRY", MEASURED WITH X-RAYS IN CALCITE. By W.
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It is well known (in both Bragg and Laue cases) that the
relationship between the wave field produced in a
perfect crystal and the lattice depends directly on the
direction of the incident wave. In most cases (e.g. in
all reflections of monoatomic crystals), refraction and
absorption increase with increasing diffraction angle
("Prins-Kohler asymmetry"). If, however, polyatomic
crystals contain atoms with strongly different scat-
tering and absorption powers, the inverse can happen:
decreasing absorption with increasing scattering angle
leads to the "inverse absorption asymmetry". This has
been predicted already in 1962 by G. Borrmann (Z.Kri-
stallogr.120(1964)143,and J.M.Cowley recommended to use
the 222 planes in calcite or the 110 planes in sodium
nitrate for an experimental proof; but using the Laue
case, he found a clear indication of the effect only
with NaNO$_3$ (Acta Crystallogr. 17(1964)33).
As mentioned elsewhere in this volume (Fiedler, Heyer,
Hildebrandt, Jähnig) we used a double crystal diffracto-
meter with a somewhat unconventional design for the
detection of the above effect in highly perfect calcite
crystals in the Bragg case (222 reflection, CuK$_\alpha$ radi-
ation). These crystals were selected using surface to-
pographical methods (Berg-Barrett, Lang, Double
Crystal); artificial 111 and 655 surfaces were prepared
by grinding and etch-pit-free etching with diluted (2%)
CP 4.
Considering symmetrical and asymmetrical reflections,
there exist nine possible (n;-n) arrangements (net
planes of the crystals nearly parallel); in three pairs,
however, FWHM and shape are predicted to be the same,
only the percent reflection differs. Out of the six re-
maining configurations, three are suited to reveal the
diffraction pattern of the test crystal: high resolu-
tion together with high intensity offers the quasi-dis-
persion-free V-S-arrangement (Renninger's notation:
crystal I with grazing incidence, crystal II in symme-
trical reflection), whereas the other two settings show a
small dispersion effect due to the different refraction
by the crystals, depending on the amount of asymmetry.
Using the crystal with a 655 surface as crystal I, the
asymmetry factor is b=-0.055 (with θ_{222}=15.76^0 and the
asymmetry angle 14.18^0). With a symmetrical 222 reflec-
tion at crystal II, a diffraction pattern with a FWHM of
2.15" and a percent reflection of 63% should result; the
measured values were 2.88" and 48%, resp., the discre-
pancy probably being due to crystal defects. The integra-
ted intensity, however, agreed to 1.2% to the expected
theoretical value (comparable to Renninger's results on
the cleavage plane (211); Acta Cryst.8(1955)597).
In Fig.1 the measured pattern (curve with points) is
compared to a calculated one, which results from a re-
duction of the theoretical pattern to 48% reflectivity,
keeping the integrated intensity constant. The asymmetry
lies clearly on the correct side; this is even more evi-
dent if the measured pattern is reflected at an ordinate
traversing the maximum (Fig.2). Therefore these measu-
rements yield a clear evidence of the expected effect,
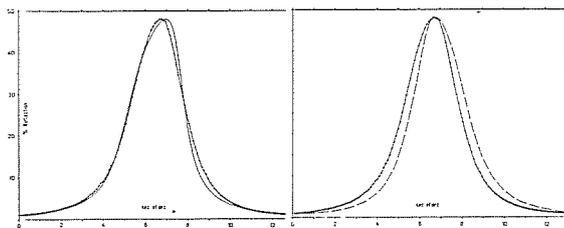
11.7—22   THE ANGULAR DEPENDENCE OF ATOMIC X-RAY DIS-
PERSION CORRECTIONS. By G. Hildebrandt, J. Kühn, Fritz-
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X-ray dispersion corrections have been calculated in
the past by several authors using different theoretical
approaches. In addition, there are now a number of ex-
perimental determinations of dispersion corrections
which allow comparison with the theoretical data. A
critical issue is the angular dependence of dispersion
corrections. Although the theoretical treatment for the
calculation of this dependence is correctly presented
in I.Waller's paper (Z.Phys. 51 (1927) 213) on the
dispersion of x-rays in atoms and has been calculated
by H.Hönl (Ann.Phys. (5) 18 (1933) 625) accordingly
for the K-shell of atoms, not much notice has been
taken by some authors who attempt to calculate this
angular dependence. They simply multiplied the oscilla-
tor strengths for dipole transitions by the correspond-
ing electron form factor (i.e. the Fourier transform of
the electron charge distribution) for the electron in
consideration, (Prins,J.A.: Z.Phys. 63 (1930) 477(for-
mula 9 page 428); Zachariasen,W.H.: Theory of X-Ray
Diffraction in Crystals (formula 3.31, page 96) Dover
Publ. Inc., New York 1967; James,R.W.: The Optical
Principles of the Diffraction of X-Rays (formula 6.47,
page 324), Bell and Sons Ltd., London 1962). Waller's
formula shows that the angular dependence in the "ano-
malous dispersion" term is, apart from the Lorentz
factor (i.e. the polarization factor), only due to the
retardation terms in the atomic transition matrix ele-
ments for the in- and outgoing x-rays. Retardation
effects are neglected in the dipole approximation
since the retardation factors are put equal to one. The
"dipole" dispersion corrections are therefore not angu-
lar dependent. The second term in a Taylor expansion of
the retardation factors corresponds to "quadrupole"
transitions.
The corresponding dispersion corrections depend on the
scattering angle and the wave length independently.
These terms are small relative to dipole terms. One of
us (Wagenfeld,H.K.: Theoretical computations of x-ray
dispersion corrections. In: Anomalous Scattering, Ed.
S.Ramaseshan and S.C.Abrahams, IUCr, Munksgaard, Copen-
hagen 1975) pointed this out at the conference on
anomalous scattering in Madrid (1974) where numerical
calculations of anomalous dispersion terms and their
angular dependence have been reported; however in-
correct numerical results were included in the final
publication of the conference proceedings (Hazel,A.C.,
pp. 48-50 in: Anomalous Scattering, see above). False
assumptions concerning the angular dependence can lead
to significant errors in some structure determinations.
The points mentioned in the manuscript presented in
Madrid, however, are well accepted by scientists work-
ing in the field of dynamical x-ray diffraction on
perfect crystals, and the theoretical data have been,
in some cases, experimentally confirmed. We will now
present revised numerical dispersion data for different
elements, x-ray wave lengths, and scattering angles
based on an extended Hönl calculation.

Fig. 1   Fig. 2

Theory ———— ; meas. ++++ ; meas.(refl.) — — — —.