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Ferroelectric Space Groups

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Abstract

The 440 ferroelectric space groups, *viz* the Heesch–Shubnikov (magnetic) space groups, which are symmetry groups of ferroelectric electric-dipole arrangements in crystals, are derived and tabulated. By considering automorphisms induced by the automorphisms of the discrete space-time group, we show that although ferroelectric, ferromagnetic and ferrocurrent point groups all number 31, the number of ferroelectric space groups differs from 275, which is that of both ferromagnetic and ferrocurrent space groups.

I. Introduction

Which of the 1651 Heesch–Shubnikov (magnetic) space groups are ferroelectric space groups, that is, symmetry groups of ferroelectric electric-dipole arrangements in crystals? Neronova & Belov (1960) have tabulated a list of 275 Heesch–Shubnikov space groups, which they call ferroelectric space groups. These authors, however, do not take into account the fact that the action of elements of Heesch-Shubnikov groups on a polarization P cannot be arbitrarily defined within the usual electromagnetic theory based on Maxwell's equations. Their choice of action is incompatible with that theory and consequently their list of 275 Heesch–Shubnikov space groups is not that of the ferroelectric space groups. With a choice of action that is compatible with that theory, Cracknell (1975) has stated that the number of ferroelectric space groups is 275, Schwarzenberger (1984) gives it as 265. No tabulation is given by either of these authors.

In § II we shall review the action of the discrete space-time group on electromagnetic quantities. We then derive and tabulate the 440 ferroelectric space groups-the Heesch-Shubnikov space groups that are symmetry groups of ferroelectric electric-dipole arrangements in crystals. In § III we discuss why, although the same number, 31, is the number of ferroelectric, ferromagnetic and ferrocurrent point groups, the number of ferroelectric space groups is different from the number, 275, of both ferromagnetic and ferrocurrent space groups.

II. Ferroelectric space groups

Let $\mathcal{U} = 1, \bar{1}, 1', \bar{1}'$ denote the discrete space-time group consisting of the identity 1, space inversion $\bar{1}$, time inversion $1'$, and $\bar{1}'$, the product of space inversion and time inversion. Further, let P, M, J and ρ denote the four quantities polarization, magnetization, current density and charge density, respectively, that appear in Maxwell's equations. These quantities can be classified according to the symmetry operations that are the elements of $\mathcal{U}$ (Ascher, 1966). In Table 1 we give the character table of $\mathcal{U}$ and classify the four quantities that appear in Maxwell's equations according to irreducible representations of the group $\mathcal{U}$. This classification and the symmetry operations of $\mathcal{U}$ on these quantities follows from the assumption that the charge density is invariant under $\mathcal{U}$ and the covariance of Maxwell's equations under $\mathcal{U}$ (Opechowski, 1985).

Table 1. *Character table of the discrete space-time group* $\mathcal{U}$

Basis functions of the irreducible representations, on the right, are given in terms of the charge density ρ and the components of polarization P, magnetization M and current density J.

1	$\bar{1}$	$1'$	$\bar{1}'$	
1	1	1	1	ρ
1	−1	1	−1	P_x, P_y, P_z
1	1	−1	−1	M_x, M_y, M_z
1	−1	−1	1	J_x, J_y, J_z

Table 2. *The thirty-one ferroelectric point groups*

1	1′		
2	21′	2′	
m	*m*1′	*m*′	
*mm*2	*mm*21′	*m*′*m*′2	*m*′*m*2′
3	31′		
3*m*	3*m*1′	3*m*′	
4	41′	4′	
4*mm*	4*mm*1′	4*m*′*m*′	4′*m*′*m*
6	61′	6′	
6*mm*	6*mm*1′	6*m*′*m*′	6′*m*′*m*

It follows from Table 1 and the vector properties of P, M and J that the maximal symmetry group of a polarization vector P is $\infty m1'$, of a magnetization vector M, $\infty/m\,m'$, and of a current density vector J, $\infty/m'\,m$. To determine which Heesch–Shubnikov groups are ferroelectric space groups, one determines which Heesh–Shubnikov groups have a point group that is a subgroup of $\infty m1'$. (In a similar manner one finds all ferromagnetic and ferrocurrent space groups by determining which Heesch–Shubnikov groups have a point group that is a subgroup of $\infty/m\,m'$ or

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Table 3. *The four hundred and forty ferroelectric space groups*

The table is subdivided into subtables, all groups in one subtable having the same point group listed at the top of the subtable. We list the groups in the notation of Opechowski & Guccione (1965) and, if it is different, on the right give the notation of Belov, Neronova & Smirnova (1957).

1

$P1$

1'

$P_{2s}1$	P_s1
$P11'$	

2

$P2$
$P2_1$
$C2$

21'

$P_{2a}2$	P_a2
$P_{2b}2$	P_b2
P_C2	C_a2
$P_{2b}2'$	P_b2_1
$P_{2a}2_1$	P_a2_1
$C_{2c}2$	C_c2
C_P2	P_C2
C_P2'	P_C2_1
$P21'$	
$P2_11'$	
$C21'$	

2'

$P2'$
$P2_1'$
$C2'$

m

Pm
Pc
Cm
Cc

m1'

$P_{2a}m$	P_am
$P_{2b}m$	P_bm
P_Cm	C_am
$P_{2c}m'$	P_cc
$P_{2a}c$	P_ac
$P_{2b}c$	P_bc
P_Cc	C_ac
$C_{2c}m$	C_cm
C_Pm	P_Cm
$C_{2c}m'$	C_cc
C_Pm'	P_Ac
C_Pc	P_Cc
$Pm1'$	
$Pc1'$	
$Cm1'$	
$Cc1'$	

m'

Pm'
Pc'
Cm'
Cc'

mm2

$Pmm2$
$Pmc2_1$
$Pcc2$
$Pma2$
$Pca2_1$
$Pnc2$
$Pmn2_1$
$Pba2$
$Pna2_1$
$Pnn2$
$Cmm2$
$Cmc2_1$
$Ccc2$
$Amm2$
$Abm2$
$Ama2$
$Aba2$
$Fmm2$
$Fdd2$
$Imm2$
$Iba2$
$Ima2$

mm21'

$P_{2c}mm2$	P_cmm2
$P_{2a}mm2$	P_amm2
P_Cmm2	C_amm2
P_Amm2	A_cmm2
P_Fmm2	F_smm2
$P_{2c}mm'2'$	P_cmc2_1
$P_{2c}m'm'2$	P_ccc2
$P_{2a}m'm'2$	P_ama2
$P_Am'm'2$	A_cbm2
$P_{2a}mc2_1$	P_amc2_1
$P_{2b}mc2_1$	P_bmc2_1
P_Cmc2_1	C_amc2_1
$P_{2a}mc'2_1'$	P_amn2_1
$P_{2b}m'c'2_1$	P_aca2_1
$P_{2a}cc2$	P_acc2
P_Ccc2	C_acc2
$P_{2b}c'c2'$	P_bnc2
$P_{2b}ma2$	P_bma2
$P_{2c}ma2$	P_cma2
P_Ama2	A_cma2
$P_{2b}m'a2'$	P_aba2
$P_{2c}m'a2'$	P_cca2_1
$P_{2c}ma'2'$	P_cmn2_1
$P_{2c}m'a'2$	P_cnc2
$P_Am'a'2$	A_cba2
$P_{2b}ca2_1$	P_bca2_1
$P_{2b}c'a'2_1$	P_bna2_1
$P_{2a}nc2$	P_anc2
$P_{2a}nc'2'$	P_ann2
$P_{2b}mn2_1$	P_bmn2_1
$P_{2b}m'n2_1'$	P_ana2_1
$P_{2c}ba2$	P_cba2
$P_{2c}b'a2'$	P_cna2_1
$P_{2c}b'a'2$	P_cnn2
P_Fnn2	F_sdd2
$C_{2c}mm2$	C_cmm2
C_Pmm2	P_cmm2
C_Imm2	I_cmm2
$C_{2c}m'm2'$	C_cmc2_1
$C_{2c}m'm'2$	C_ccc2
$C_Pm'm2'$	P_Cma2
$C_Pm'm'2$	P_Cba2
$C_Im'm2'$	I_cma2
$C_Im'm'2$	I_cba2
C_Pmc2_1	P_Cmc2_1
$C_Pm'c2_1'$	P_Cca2_1
$C_Pmc'2_1'$	P_Cmn2_1
$C_Pm'c'2_1$	P_Cna2_1
C_Pcc2	P_Ccc2
$C_Pc'c2'$	P_Cnc2
$C_Pc'c'2$	P_Cnn2
$A_{2a}mm2$	A_amm2
A_Pmm2	P_Amm2
A_Imm2	I_amm2
$A_{2a}mm'2'$	A_ama2
$A_Pm'm2'$	P_Bmn2_1
$A_Pmm'2'$	P_Amc2_1
$A_Pm'm'2$	P_Anc2
$A_Im'm'2$	I_ama2
$A_{2a}bm2$	A_abm2
A_Pbm2	P_Bma2
A_Ibm2	I_bma2
$A_{2a}b'm'2$	A_aba2
$A_Pb'm2'$	P_Bmc2_1
$A_Pbm'2'$	P_Bca2_1
$A_Pb'm'2$	P_Acc2
$A_Ib'm'2$	I_aba2
A_Pma2	P_Ama2
$A_Pm'a2'$	P_Ana2_1
$A_Pma'2'$	P_Amn2_1
$A_Pm'a'2$	P_Ann2
A_Pba2	P_Aba2
$A_Pb'a2'$	P_Aca2_1
$A_Pba'2'$	P_Bna2_1
$A_Pb'a'2$	P_Bnc2
F_Cmm2	C_Amm2
F_Amm2	A_Cmm2
$F_Cmm'2'$	C_Amc2_1
$F_Cm'm'2$	C_Acc2
$F_Am'm2'$	A_Cbm2
$F_Amm'2'$	A_Cma2
$F_Am'm'2$	A_Cba2
I_Pmm2	P_Imm2
$I_Pmm'2'$	P_Imn2_1
$I_Pm'm'2$	P_Inn2
I_Pba2	P_Icc2
$I_Pba'2'$	P_Ica2_1
$I_Pb'a'2$	P_Iba2
I_Pma2	P_Ima2
$I_Pm'a2'$	P_Ina2_1
$I_Pma'2'$	P_Imc2_1
$I_Pm'a'2$	P_Inc2
$Pmm21'$	
$Pmc2_11'$	
$Pcc21'$	
$Pma21'$	
$Pca2_11'$	
$Pnc21'$	
$Pmn2_11'$	
$Pba21'$	
$Pna2_11'$	
$Pnn21'$	
$Cmm21'$	
$Cmc2_11'$	
$Ccc21'$	
$Amm21'$	
$Abm21'$	
$Ama21'$	
$Aba21'$	
$Fmm21'$	
$Fdd21'$	
$Imm21'$	
$Iba21'$	
$Ima21'$	

m'm2'

$Pm'm2'$
$Pm'c2_1'$
$Pmc'2_1'$
$Pc'c2'$
$Pm'a2'$
$Pma'2'$
$Pc'a2_1'$
$Pca'2_1'$
$Pn'c2'$
$Pnc'2'$
$Pm'n2_1'$
$Pmn'2_1'$
$Pb'a2'$
$Pn'a2_1'$
$Pna'2_1'$
$Pn'n2'$
$Cm'm2'$
$Cm'c2_1'$
$Cmc'2_1'$
$Cc'c2'$
$Am'm2'$
$Amm'2'$
$Ab'm2'$
$Abm'2'$
$Am'a2'$
$Ama'2'$
$Ab'a2'$
$Aba'2'$
$Fm'm2'$
$Fd'd2'$
$Im'm2'$
$Ib'a2'$
$Im'a2'$
$Ima'2'$

3

$P3$
$P3_1$
$P3_2$
$R3$

31'

$P_{2c}3$	P_c3
$P_{2c}3_2$	P_c3_2
$P_{2c}3_1$	P_c3_1
R_R3	R_I3
$P31'$	
$P3_11'$	
$P3_21'$	
$R31'$	

3m

$P3m1$
$P31m$
$P3c1$
$P31c$
$R3m$
$R3c$

3m1'

$P_{2c}3m1$	P_c3m1
$P_{2c}3m'1$	P_c3c1
$P_{2c}31m$	P_c31m
$P_{2c}31m'$	P_c31c
R_R3m	R_I3m
R_R3m'	R_I3c
$P3m11'$	
$P31m1'$	
$P3c11'$	
$P31c1'$	
$R3m1'$	
$R3c1'$	

3m'

$P3m'1$
$P31m'$
$P3c'1$
$P31c'$
$R3m'$
$R3c'$

4

$P4$
$P4_1$
$P4_2$
$P4_3$
$I4$
$I4_1$

41'

$P_{2c}4$	P_c4
P_P4	P_C4
P_I4	I_c4
$P_{2c}4'$	P_c4_2
P_P4_1	P_C4_1
$P_{2c}4_2$	P_c4_1
P_P4_2	P_C4_2
P_I4_2	I_c4_1
$P_{2c}4_2'$	P_c4_3
P_P4_3	P_C4_3
I_P4	P_I4
I_P4'	P_I4_2
I_P4_1	P_I4_1
I_P4_1'	P_I4_3
$P41'$	
$P4_11'$	
$P4_21'$	
$P4_31'$	
$I41'$	
$I4_11'$	

4'

$P4'$
$P4_1'$
$P4_2'$
$P4_3'$
$I4'$
$I4_1'$

4mm

$P4mm$
$P4bm$
$P4_2cm$
$P4_2nm$
$P4cc$
$P4nc$
$P4_2mc$
$P4_2bc$
$I4mm$
$I4cm$
$I4_1md$
$I4_1cd$

4mm1'

$P_{2c}4mm$	P_c4mm
P_P4mm	P_C4mm
P_I4mm	I_c4mm
$P_{2c}4'm'm$	P_c4_2cm
$P_{2c}4'mm'$	P_c4_2mc
$P_{2c}4m'm'$	P_c4cc
$P_P4'mm'$	P_C4bm
$P_I4m'm'$	I_c4cm
$P_{2c}4bm$	P_c4bm
$P_{2c}4'b'm$	P_c4_2nm
$P_{2c}4'bm'$	P_c4_2bc
$P_{2c}4b'm'$	P_c4nc
P_P4_2cm	P_C4_2mc
$P_P4_2'cm'$	P_C4_2bc
P_I4_2nm	I_c4_1md
$P_I4_2n'm'$	I_c4_1cd
P_P4cc	P_C4cc
$P_P4'cc'$	P_C4nc
P_P4_2mc	P_C4_2cm
$P_P4_2'mc'$	P_C4_2nm
I_P4mm	P_I4mm
$I_P4'm'm$	P_I4_2nm
$I_P4'mm'$	P_I4_2mc
$I_P4m'm'$	P_I4nc
I_P4cm	P_I4bm
$I_P4'c'm$	P_I4_2cm
$I_P4'cm'$	P_I4_2bc
$I_P4c'm'$	P_I4cc
$P4mm1'$	
$P4bm1'$	
$P4_2cm1'$	
$P4_2nm1'$	
$P4cc1'$	
$P4nc1'$	
$P4_2mc1'$	
$P4_2bc1'$	
$I4mm1'$	
$I4cm1'$	
$I4_1md1'$	
$I4_1cd1'$	

4m'm'

$P4m'm'$
$P4b'm'$
$P4_2c'm'$
$P4_2n'm'$
$P4c'c'$
$P4n'c'$
$P4_2m'c'$
$P4_2b'c'$
$I4m'm'$
$I4c'm'$
$I4_1m'd'$
$I4_1c'd'$

4'm'm

$P4'm'm$
$P4'mm'$
$P4'b'm$
$P4'bm'$
$P4_2'c'm$
$P4_2'cm'$
$P4_2'n'm$
$P4_2'nm'$
$P4'c'c$
$P4'cc'$
$P4'n'c$
$P4'nc'$
$P4_2'm'c$
$P4_2'mc'$
$P4_2'b'c$
$P4_2'bc'$
$I4'm'm$
$I4'mm'$
$I4'c'm$
$I4'cm'$
$I4_1'm'd$
$I4_1'md'$
$I4_1'c'd$
$I4_1'cd'$

6

$P6$
$P6_1$
$P6_5$
$P6_2$
$P6_4$
$P6_3$

61'

$P_{2c}6$	P_c6
$P_{2c}6'$	P_c6_3
$P_{2c}6_2$	P_c6_1
$P_{2c}6_2'$	P_c6_4
$P_{2c}6_4$	P_c6_2
$P_{2c}6_4'$	P_c6_5
$P61'$	
$P6_11'$	
$P6_51'$	
$P6_21'$	
$P6_41'$	
$P6_31'$	

6'

$P6'$
$P6_1'$
$P6_5'$
$P6_2'$
$P6_4'$
$P6_3'$

6mm

$P6mm$
$P6cc$
$P6_3cm$
$P6_3mc$

6mm1'

$P_{2c}6mm$	P_c6mm
$P_{2c}6'm'm$	P_c6_3cm
$P_{2c}6'mm'$	P_c6_3mc
$P_{2c}6m'm'$	P_c6cc
$P6mm1'$	
$P6cc1'$	
$P6_3cm1'$	
$P6_3mc1'$	

6m'm'

$P6m'm'$
$P6c'c'$
$P6_3c'm'$
$P6_3m'c'$

6'm'm

$P6'm'm$
$P6'mm'$
$P6'c'c$
$P6'cc'$
$P6_3'c'm$
$P6_3'cm'$
$P6_3'm'c$
$P6_3'mc'$

Table 4. *Automorphisms of the discrete space–time group* $\mathcal{U}$

An element in the ith row of the left-hand column is mapped under the automorphism A_j in the jth column of the top row into the element of $\mathcal{U}$ at the intersection of the ith row and jth column.

	A_0	A_1	A_2	A_3	A_4	A_5
1	1	1	1	1	1	1
$\bar{1}$	$\bar{1}$	$\bar{1}$	$\bar{1}'$	$1'$	$\bar{1}'$	$1'$
$1'$	$1'$	$\bar{1}'$	$1'$	$\bar{1}$	$\bar{1}$	$\bar{1}'$
$\bar{1}'$	$\bar{1}'$	$1'$	$\bar{1}$	$\bar{1}'$	$1'$	$\bar{1}$

Table 5. *The set of all ferroelectric (FE), ferromagnetic (FM) or ferrocurrent (FC) point groups given in the ith row of the left-hand column is mapped under the automorphism A_j in the jth column of the top row into a set of FE, FM or FC point groups according to the entry at the intersection of the ith row and jth column*

	A_0	A_1	A_2	A_3	A_4	A_5
FE	FE	FC	FE	FM	FM	FC
FM	FM	FM	FC	FE	FC	FE
FC	FC	FE	FM	FC	FE	FM

$\infty/m'm$.) The point groups of Heesch–Shubnikov groups that are subgroups of $\infty m1'$–the ferroelectric point groups–are listed in Table 2.

In Table 3 we list the 440 ferroelectric space groups. These are all the Heesch–Shubnikov groups whose point group is one of the ferroelectric groups (listed in Table 2). Table 3 has been subdivided into subtables, all ferroelectric groups with the same ferroelectric point group appearing in one subtable.

There are 275 ferromagnetic space groups (Neronova Belov, 1960; Opechowski & Guccione, 1965) and 275 ferrocurrent space groups. The latter have been listed by Neronova & Belov (1960) but are called by them ferroelectric space groups. This nomenclature is incompatible with the usual electromagnetic theory based on Maxwell's equations, and is misleading as it does not give the correct number of ferroelectric space groups. Of the 440 ferroelectric space groups listed in Table 3, 68 are non-magnetic space groups F, 68 are of the form $F1'$ and, using the notation of Opechowski & Guccione (1965), 129 are magnetic groups M_T and175 are magnetic groups M_R. We note that the sum of the first three types is 265, the number of ferroelectric space groups given by Schwarzenberger (1984).

III. Numerology

There are 31 ferroelectric point groups, 31 ferromagnetic point groups and 31 ferrocurrent point groups (Ascher, 1966; Cracknell, 1972; Kopsky, 1976; Ascher & Janner, undated). There are 275 ferromagnetic space groups, 275 ferrocurrent space groups and 440 ferroelectric space groups. To understand why the number of ferroelectric, ferromagnetic and ferrocurrent point groups is the same, and why the number of ferromagnetic and ferrocurrent space groups is the same, though different from that of ferroelectric space groups, requires considering the automorphisms of the discrete space–time group $\mathcal{U}$.

The six automorphisms A_1, $i = 0, 1, 2, 3, 4, 5$, of the discrete space–time group $\mathcal{U}$ are listed in Table 4 (Kopsky, 1976). These automorphisms of $\mathcal{U}$ induce automorphisms of the group $R_+(3) \times \mathcal{U}$, where $R_+(3)$ is the group of all proper three-dimensional rotations: Let $A_i[u]$ denote the element of $\mathcal{U}$ into which the element u of $\mathcal{U}$ is mapped under the automorphism A_i. The mapping $A_i[R_+u] = R_+A_i[u]$ then defines an automorphism of $R_+(3) \times \mathcal{U}$. Under these automorphisms of $R_+(3) \times \mathcal{U}$, the set of all ferroelectric point groups is mapped into sets of point groups, which, depending on the automorphism A_i, are sets of distinct ferroelectric, ferromagnetic or ferrocurrent point groups. The same is true for the set of all ferromagnetic point groups and the set of all ferrocurrent point groups. In Table 5 we show how each set of all ferroelectric, ferromagnetic and ferrocurrent point groups is mapped under each of the automorphisms of $R_+(3) \times \mathcal{U}$ induced by the automorphisms A_i of $\mathcal{U}$. It follows that the number of ferroelectric, ferromagnetic and ferrocurrent point groups is the same. For example, the automorphism A_2 maps the set of all ferromagnetic point groups into a set of distinct ferrocurrent point groups and simultaneously the set of all ferrocurrent point groups into a set of distinct ferromagnetic point groups. Consequently, the number of ferromagnetic and ferrocurrent point groups is the same.

However, only the identity automorphism A_0 and the automorphism A_2 of $\mathcal{U}$ induce automorphisms of the group $\mathscr{E}_+(3) \times \mathcal{U}$, where $\mathscr{E}_+(3)$ is the proper three-dimensional Euclidian group. From the automorphism induced by the automorphism A_2 of $\mathcal{U}$, it follows that the number of ferromagnetic and ferrocurrent space groups is the same. As there are no other such induced automorphisms, we conclude that the number of ferroelectric space groups may be (and, as we have shown, is) different.

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Neutron Diffraction Investigation of the Nuclear and Magnetic Extinction in MnP

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Abstract

The absolute values of the reflecting powers ρ are measured for the 200 and $2\pm\tau$,0,0 set of magnetic and nuclear reflections in the helimagnetic phase of a good-quality crystal of MnP as a function of its thickness. Severe and very different extinction effects are observed for the magnetic and nuclear reflections ($y_{\rm magnetic}\sim 0{\cdot}4$, $y_{\rm nuclear}\sim 0{\cdot}02$ for the largest thickness). This corresponds to the spectacular result that the magnetic reflecting powers $\rho_\pm$ are twice as big as the nuclear one ρ_N, in spite of the fact that the scattering cross sections $|F_\pm|^2$ are about ten times smaller than the nuclear $|F_N|^2$. The nuclear results appear consistent with dynamical theory while the magnetic ones are not. They can be explained by Zachariasen's type II secondary extinction model based on the chirality domain pattern. The same measurements were performed in the ferromagnetic phase, yielding $y_{\rm ferro}\simeq 0{\cdot}03$. A model using the relative sizes of the ferromagnetic and chirality domains is presented.

I. Introduction

The basic publication on extinction for the neutron case, within the framework of the mosaic model, is now nearly forty years old (Bacon & Lowde, 1948). Since then most of the improvements introduced to correct the extinction of the intensities diffracted by a single-crystal sample originate from the theory based on the Darwin energy transfer equations worked out by Zachariasen (1967). This theory was modified to take into account the anisotropy of the extinction by Coppens & Hamilton (1970) and Thornley & Nelmes (1974). The formalism was reconsidered and improved by Cooper & Rouse (1970) and Becker & Coppens (1974*a*, *b*) in order to apply it to spherical or ellipsoidal crystals, the theory being extended to non-spherical crystals with anisotropic extinction by Becker & Coppens (1975).

The main limitation of Zachariasen's theory is in its kinematical approach to the scattering, as pointed out by Werner (1969, 1974): the coherence of the transmitted and diffracted beams is not taken into account, and so this method does not appear to be suitable for correction for severe primary extinction. Another approach, starting from the dynamical theory of diffraction, was worked out for distorted crystals by several authors (Klar & Rustichelli, 1973; Gronkowski & Malgrange, 1984; Kulda, 1984), but mainly by Kato (1976), who has partially reconciled the two approaches. He shows that for optical coherence lengths smaller than the extinction distance Λ the new treatment leads to the usual coupling equations. Kato (1980) has also developed a consistent statistical theory of extinction covering the whole range of crystal quality from perfect (dynamical theory) to ideally imperfect (kinematical approximation). The results of this last theory have recently been compared to those of previous ones (Becker & Dunstetter, 1984) and experimentally tested using polarized neutrons (Guigay, Schlenker, Baruchel & Schweizer, unpublished).

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