

1. GENERAL RELATIONSHIPS AND TECHNIQUES

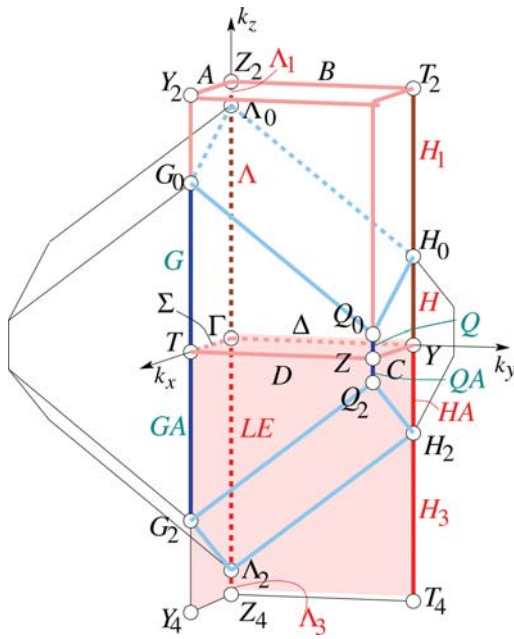


Fig. 1.5.5.6. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $mm2F$: $c^{-2} > a^{-2} + b^{-2}$. Space groups $Fmm2 - C_{2v}^{18}$ (42), $Fdd2 - C_{2v}^{19}$ (43). Reciprocal-space group $(Imm2)^*$, No. 44: $c^{*2} > a^{*2} + b^{*2}$ (see Table 1.5.5.6). The representation domain of CDML is different from the asymmetric unit. Auxiliary points: T_4 : $0, \frac{1}{2}, -\frac{1}{2}$; Y_4 : $\frac{1}{2}, 0, -\frac{1}{2}$; Z_4 : $0, 0, -\frac{1}{2}$. Flagpoles: $0, 0, z$: $-\frac{1}{2} < z < 0$; $0, \frac{1}{2}, z$: $-\frac{1}{2} < z < 0$. Wings: $x, 0, z$: $0 < x < \frac{1}{2}, -\frac{1}{2} < z < 0$; $0, y, z$: $0 < y < \frac{1}{2}, -\frac{1}{2} < z < 0$.

In general the sequence of the Wyckoff letters in IT A follows the falling number of free parameters. In the few cases where the sequence in IT A is different, the Wyckoff letters are exchanged. The exchange is noted at the top of the table.

Example. In the arithmetic crystal class $4/mmmI$, $c/a < 1$, see Table 1.5.5.3, Wyckoff position e has one free parameter, whereas Wyckoff position f has constant parameters, i.e. no free parameter. Therefore, f is listed above the horizontal line, e is listed below, see Table 1.5.5.3. The note at the top of the table states ‘Wyckoff positions e and f exchanged’.

Parameter relations. The relations between the parameters of CDML and the parameters referred to the asymmetric unit are listed at the top of the table, e.g. for $m\bar{3}mI$ in Table 1.5.5.1: ‘Parameter relations: $x = \frac{1}{2}\beta + \frac{1}{2}\gamma$, $y = \frac{1}{2}\alpha + \frac{1}{2}\gamma$, $z = \frac{1}{2}\alpha + \frac{1}{2}\beta$ ’. These relations may be modified to more convenient parameters without notice, as for the plane B of $m\bar{3}mI$ in Table 1.5.5.1:

$$B \quad \alpha + \beta, -\alpha + \beta, \frac{1}{2} - \beta \quad ex \quad 96 \quad k \quad ..m \quad x, \frac{1}{2} - x, z: 0 < z < x < \frac{1}{4}$$

instead of

$$\dots \frac{1}{4} - \frac{1}{2}\alpha, \frac{1}{4} + \frac{1}{2}\alpha, \beta: 0 < \alpha < \frac{1}{2} - 2\beta < \frac{1}{2}.$$

1.5.5.3. Figures and tables

Arithmetic crystal classes $m\bar{3}mI$ and $m\bar{3}I$: The reciprocal lattice of a cubic lattice I is a cubic lattice F . Its Brillouin zone is a rhombic dodecahedron and has 12 faces, 24 edges and 14 apices, the coordinates of which are the six permutations of $\pm\frac{1}{2}, 0, 0$ and the eight coordinate triplets of $\pm\frac{1}{4}, \pm\frac{1}{4}, \pm\frac{1}{4}$. Eleven of these 14 points are visible in the applied projection.

Table 1.5.5.6. List of k -vector types for arithmetic crystal class $mm2F$: $c^{-2} > a^{-2} + b^{-2}$

See Fig. 1.5.5.6. Parameter relations: $x = -\frac{1}{2}\alpha + \frac{1}{2}\beta + \frac{1}{2}\gamma$, $y = \frac{1}{2}\alpha - \frac{1}{2}\beta + \frac{1}{2}\gamma$, $z = \frac{1}{2}\alpha + \frac{1}{2}\beta - \frac{1}{2}\gamma$.

k -vector label, CDML	Wyckoff position of IT A, cf. Section 1.5.4.3	Parameters
Γ 0, 0, 0	ex 2 a $mm2$	0, 0, 0
Z $\frac{1}{2}, \frac{1}{2}, 1$	ex 2 a $mm2$	$\frac{1}{2}, \frac{1}{2}, 0$ $0, 0, \frac{1}{2}$
$Z \sim Z_2$		
Λ $\alpha, \alpha, 0$	ex 2 a $mm2$	$0, 0, z: 0 < z \leq \lambda_0$
LE $-\alpha, -\alpha, 0$	ex 2 a $mm2$	$0, 0, z: \lambda_2 = -\lambda_0 < z < 0$
Q $\frac{1}{2} + \alpha, \frac{1}{2} + \alpha, 1$	ex 2 a $mm2$	$\frac{1}{2}, \frac{1}{2}, z: 0 < z \leq q_0$ $0, 0, z: -\frac{1}{2} < z \leq -\frac{1}{2} + q_0 = -\lambda_0$
$Q \sim \Lambda_3 = [\Lambda_2 Z_4]$		
QA $\frac{1}{2} - \alpha, \frac{1}{2} - \alpha, 1$	ex 2 a $mm2$	$\frac{1}{2}, \frac{1}{2}, z: q_2 = -q_0 < z < 0$
$QA \sim \Lambda_1 = [\Lambda_0 Z_2]$		
$Z_2 \cup \Lambda_1 \cup \Lambda \cup \Gamma \cup LE \cup \Lambda_3$	2 a $mm2$	$0, 0, z: \frac{1}{2} - q_0 = \lambda_0 < z < \frac{1}{2}$ $0, 0, z: -\frac{1}{2} < z \leq \frac{1}{2}$
T $0, \frac{1}{2}, \frac{1}{2}$	ex 2 b $mm2$	$\frac{1}{2}, 0, 0$ $0, \frac{1}{2}, \frac{1}{2}$
$T \sim T_2$		
Y $\frac{1}{2}, 0, \frac{1}{2}$	ex 2 b $mm2$	$0, \frac{1}{2}, 0$
G $\alpha, \frac{1}{2} + \alpha, \frac{1}{2}$	ex 2 b $mm2$	$\frac{1}{2}, 0, z: 0 < z \leq g_0$ $0, \frac{1}{2}, z: -\frac{1}{2} < z \leq -\frac{1}{2} + g_0$
$G \sim H_3 = [H_2 T_4]$		
GA $-\alpha, \frac{1}{2} - \alpha, \frac{1}{2}$	ex 2 b $mm2$	$\frac{1}{2}, 0, z: g_2 = -g_0 < z < 0$ $0, \frac{1}{2}, z: \frac{1}{2} - g_0 = h_0 < z < \frac{1}{2}$
$GA \sim H_1 = [H_0 T_2]$		
H $\frac{1}{2} + \alpha, \alpha, \frac{1}{2}$	ex 2 b $mm2$	$0, \frac{1}{2}, z: 0 < z \leq h_0$
HA $\frac{1}{2} - \alpha, -\alpha, \frac{1}{2}$	ex 2 b $mm2$	$0, \frac{1}{2}, z: h_2 = -h_0 < z < 0$
$T_2 \cup H_1 \cup H \cup Y \cup HA \cup H_3$	2 b $mm2$	$0, \frac{1}{2}, z: -\frac{1}{2} < z \leq \frac{1}{2}$
Σ 0, α , α	ex 4 c $.m$.	$x, 0, 0: 0 < x < \frac{1}{2}$
C $\frac{1}{2}, \alpha, \frac{1}{2} + \alpha$	ex 4 c $.m$.	$x, \frac{1}{2}, 0: 0 < x < \frac{1}{2}$ $x, 0, \frac{1}{2}: 0 < z < \frac{1}{2}$
$C \sim A = [Z_2 Y_2]$		
J $\alpha, \alpha + \beta, \beta$	ex 4 c $.m$.	$x, 0, z: [\Gamma \Lambda_0 G_0 T]$
JA $-\alpha, -\alpha + \beta, \beta$	ex 4 c $.m$.	$x, 0, z: [\Gamma T G_2 \Lambda_2]$
K $\frac{1}{2} + \alpha, \alpha + \beta, \frac{1}{2} + \beta$	ex 4 c $.m$.	$x, \frac{1}{2}, z: [Y H_0 Q_0 Z]$
$K \sim J_3$		
KA $\frac{1}{2} - \alpha, -\alpha + \beta, \frac{1}{2} + \beta$	ex 4 c $.m$.	$x, 0, z: [Y_4 G_2 \Lambda_2 Z_4]$ $x, \frac{1}{2}, z: [Z Q_2 H_2 Y]$
$KA \sim J_1$		
$A \cup J_1 \cup J \cup \Sigma \cup JA \cup J_3$	4 c $.m$.	$x, 0, z: 0 < x < \frac{1}{2}, -\frac{1}{2} < z \leq \frac{1}{2}$
Δ $\alpha, 0, \alpha$	ex 4 d $m..$	$0, y, 0: 0 < y < \frac{1}{2}$
D $\alpha, \frac{1}{2}, \frac{1}{2} + \alpha$	ex 4 d $m..$	$\frac{1}{2}, y, 0: 0 < y < \frac{1}{2}$ $0, y, \frac{1}{2}: 0 < y < \frac{1}{2}$
$D \sim B$		
E $\alpha + \beta, \alpha, \beta$	ex 4 d $m..$	$0, y, z: [\Gamma Y H_0 \Lambda_0]$
EA $-\alpha + \beta, -\alpha, \beta$	ex 4 d $m..$	$0, y, z: [\Gamma \Lambda_2 H_2 Y]$
F $\alpha + \beta, \frac{1}{2} + \alpha, \frac{1}{2} + \beta$	ex 4 d $m..$	$\frac{1}{2}, y, z: [T Z Q_0 G_0]$ $0, y, z: [Z_4 \Lambda_2 H_2 T_4]$
$F \sim E_3$		
FA $-\alpha + \beta, \frac{1}{2} - \alpha, \frac{1}{2} + \beta$	ex 4 d $m..$	$\frac{1}{2}, y, z: [T G_2 Q_2 Z]$ $0, y, z: [Z_2 \Lambda_0 H_0 T_2]$
$FA \sim E_1$		
$B \cup E_1 \cup E \cup \Delta \cup EA \cup E_3$	4 d $m..$	$0, y, z: 0 < y < \frac{1}{2}, -\frac{1}{2} < z \leq \frac{1}{2}$
GP α, β, γ	8 e 1	$x, y, z: 0 < x, y < \frac{1}{2}, 0 < z \leq \frac{1}{2}$

The figure for arithmetic crystal class $m\bar{3}mI$ is shown in Fig. 1.5.5.1 and the corresponding table is Table 1.5.5.1. The figure for arithmetic crystal class $m\bar{3}I$ is shown in Fig. 1.5.5.2 and the corresponding table is Table 1.5.5.2.

Arithmetic crystal class $4/mmmI$: There are two different types of Brillouin zones for the tetragonal I lattice, one for $c < a$ (Fig. 1.5.5.3, Table 1.5.5.3) and one for $c > a$ (Fig. 1.5.5.4, Table 1.5.5.4). The first type of Brillouin zone, Fig. 1.5.5.3, is a tetragonal elongated rhombododecahedron with 12 faces, four of them being hexagons. There are 18 apices; 14 of them are visible. The Brillouin zone of Fig. 1.5.5.4 is a tetragonally deformed cuboctahedron with 14 faces. There are 24 apices; 18 of them are visible.

Arithmetic crystal class $mm2F$: Depending on the lattice ratios $a:b:c$, there are four figures in CDML for the Brillouin zone of an orthorhombic crystal with an F lattice, see Fig. 3.6 on p. 26 in CDML. Only three of them are really necessary. Therefore, the case $b^{-2} > c^{-2} + a^{-2}$ of Fig. 3.6(c) of CDML has been omitted in these examples; it is obtained from $a^{-2} > c^{-2} + b^{-2}$ of Figure 3.6(d) by a rotation by 90° about the c^* axis. The three remaining