

1.5. CLASSIFICATION OF SPACE-GROUP REPRESENTATIONS

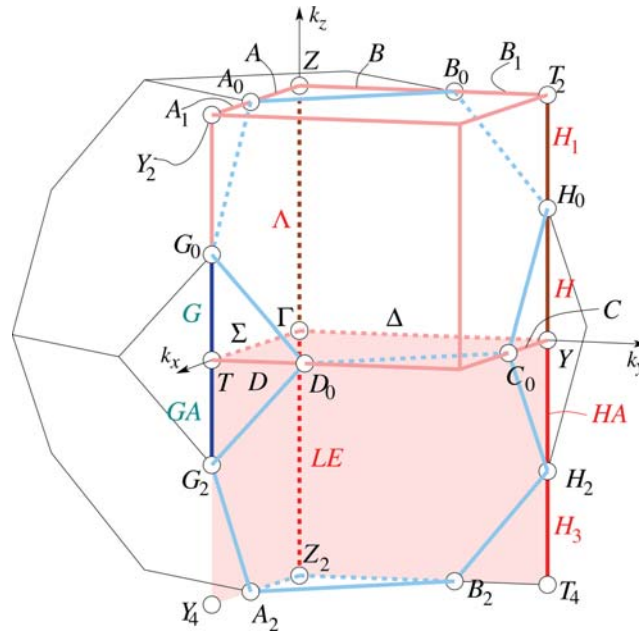


Fig. 1.5.5.5. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $mm2F$: $a^{-2} < b^{-2} + c^{-2}$, $b^{-2} < c^{-2} + a^{-2}$ and $c^{-2} < a^{-2} + b^{-2}$. Space groups $Fmm2 - C_{2v}^{18}$ (42), $Fdd2 - C_{2v}^{19}$ (43). Reciprocal-space group $(Im\bar{m}2)^*$, No. 44: $a^{*2} < b^{*2} + c^{*2}$, $b^{*2} < c^{*2} + a^{*2}$ and $c^{*2} < a^{*2} + b^{*2}$ (see Table 1.5.5.5). The representation domain of CDML is different from the asymmetric unit. Auxiliary points: T_4 : $0, \frac{1}{2}, -\frac{1}{2}$; Y_2 : $\frac{1}{2}, 0, \frac{1}{2}$; Y_4 : $\frac{1}{2}, 0, -\frac{1}{2}$; Z_2 : $0, 0, -\frac{1}{2}$. Flagpoles: $0, 0, z$: $-\frac{1}{2} < z < 0$; $0, \frac{1}{2}, z$: $-\frac{1}{2} < z < 0$. Wings: $x, 0, z$: $0 < x < \frac{1}{2}, -\frac{1}{2} < z < 0$; $0, y, z$: $0 < y < \frac{1}{2}, -\frac{1}{2} < z < 0$.

Table 1.5.5.5. List of k -vector types for arithmetic crystal class $mm2F$: $a^{-2} < b^{-2} + c^{-2}$, $b^{-2} < c^{-2} + a^{-2}$ and $c^{-2} < a^{-2} + b^{-2}$

See Fig. 1.5.5.5. 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 $\frac{1}{2}, \frac{1}{2}, 0$	ex 2 a $mm2$	$0, 0, \frac{1}{2}$
A $\alpha, \alpha, 0$	ex 2 a $mm2$	$0, 0, z$: $0 < z < \frac{1}{2}$
LE $-\alpha, -\alpha, 0$	ex 2 a $mm2$	$0, 0, z$: $-\frac{1}{2} < z < 0$
$\Gamma \cup A \cup Z \cup LE$	2 a $mm2$	$0, 0, z$: $-\frac{1}{2} < z \leq \frac{1}{2}$
T $0, \frac{1}{2}, \frac{1}{2}$	ex 2 b $mm2$	$\frac{1}{2}, 0, 0$
$T \sim T_2$		$0, \frac{1}{2}, \frac{1}{2}$
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 $mm2$	$\frac{1}{2}, 0, z$: $0 < z \leq g_0$
$G \sim H_3 = [H_2 T_4]$		$0, \frac{1}{2}, z$: $-\frac{1}{2} < z \leq -\frac{1}{2} + g_0 = h_2$
GA $-\alpha, \frac{1}{2} - \alpha, \frac{1}{2}$	ex 2 b $mm2$	$\frac{1}{2}, 0, z$: $g_2 = -g_0 < z < 0$
$GA \sim H_1 = [H_0 T_2]$		$0, \frac{1}{2}, z$: $\frac{1}{2} - g_0 = h_0 < z < \frac{1}{2}$
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 $0, \alpha, \alpha$	ex 4 c $.m.$	$x, 0, 0$: $0 < x < \frac{1}{2}$
A $\frac{1}{2}, \frac{1}{2} + \alpha, \alpha$	ex 4 c $.m.$	$x, 0, \frac{1}{2}$: $0 < x \leq a_0$
C $\frac{1}{2}, \alpha, \frac{1}{2} + \alpha$	ex 4 c $.m.$	$x, \frac{1}{2}, 0$: $0 < x < c_0 = \frac{1}{2} - a_0$
$C \sim A_1$		$x, 0, \frac{1}{2}$: $\frac{1}{2} - a_0 = c_0 < x < \frac{1}{2}$
J $\alpha, \alpha + \beta, \beta$	ex 4 c $.m.$	$x, 0, z$: $[\Gamma Z A_0 G_0 T]$
JA $-\alpha, -\alpha + \beta, \beta$	ex 4 c $.m.$	$x, 0, z$: $[\Gamma T G_2 A_2 Z_2]$
K $\frac{1}{2} + \alpha, \alpha + \beta, \frac{1}{2} + \beta$	ex 4 c $.m.$	$x, \frac{1}{2}, z$: $[Y H_0 C_0]$
$K \sim J_1$		$x, 0, z$: $[Y_4 G_2 A_2]$
KA $\frac{1}{2} - \alpha, -\alpha + \beta, \frac{1}{2} + \beta$	ex 4 c $.m.$	$x, \frac{1}{2}, z$: $[Y C_0 H_2]$
$KA \sim J_3$		$x, 0, z$: $[Y_2 G_0 A_0]$
$A \cup A_1 \cup J \cup J_3 \cup \Sigma \cup JA \cup J_1$	4 c $.m.$	$x, 0, z$: $0 < x < \frac{1}{2}, 0 < z \leq \frac{1}{2}$
Δ $\alpha, 0, \alpha$	ex 4 d $.m..$	$0, y, 0$: $0 < y < \frac{1}{2}$
B $\frac{1}{2} + \alpha, \frac{1}{2}, \alpha$	ex 4 d $.m..$	$0, y, \frac{1}{2}$: $0 < y < b_0$
D $\alpha, \frac{1}{2}, \frac{1}{2} + \alpha$	ex 4 d $.m..$	$\frac{1}{2}, y, 0$: $0 < y \leq d_0$
$D \sim B_1$		$0, y, \frac{1}{2}$: $\frac{1}{2} - d_0 = b_0 \leq y < \frac{1}{2}$
E $\alpha + \beta, \alpha, \beta$	ex 4 d $.m..$	$0, y, z$: $[\Gamma Y H_0 B_0 Z]$
EA $-\alpha + \beta, -\alpha, \beta$	ex 4 d $.m..$	$0, y, z$: $[\Gamma Z_2 B_2 H_2 Y]$
F $\alpha + \beta, \frac{1}{2} + \alpha, \frac{1}{2} + \beta$	ex 4 d $.m..$	$\frac{1}{2}, y, z$: $[T D_0 G_0]$
$F \sim E_3$		$0, y, z$: $[B_2 T_4 H_2]$
FA $-\alpha + \beta, \frac{1}{2} - \alpha, \frac{1}{2} + \beta$	ex 4 d $.m..$	$\frac{1}{2}, y, z$: $[T G_2 D_0]$
$FA \sim E_1$		$0, y, z$: $[T_2 B_0 H_0]$
$\Delta \cup B \cup B_1 \cup E \cup E_1 \cup EA \cup E_3$	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 : $0 < x, y < \frac{1}{2}, 0 < z \leq \frac{1}{2}$