

結晶学概論 第4回小テスト

Q2. LaFeAsOでCmmeの部分群Aem2へ転移したときを考える

Q. 各原子の多重度、Wyckoff letter、座標を記述し、

移動可能な座標に下線を記しなさい

注) Aem2はInt. Tbl. A1で2つあるうちの一番目

$Cmme$

No. 67

$C2/m2/m2/e$

D_{2h}^{21}

Axes

Coordinates

Wyckoff positions

$4a$	$4b$	$4c$	$4d$	$4e$	$4f$	$4g$	$8h$	$8i$	$8j$	$8k$	$8l$
									$8m$	$8n$	$16o$

I Maximal translationengleiche subgroups

[2] $C2me$ (39)			$4a$	$4b$	$4a$	$4b$	$4c$	$4c$	$4c$	$2 \times 4a$	$2 \times 4b$	$8d$	$8d$	$8d$
$\cong Aem2$	c, -b, a	$z, -y, x$										$8d$	$2 \times 4c$	$2 \times 8d$
[2] $Cm2e$ (39)		$x + \frac{1}{4}, y, z$	$4a$	$4b$	$4c$	$4c$	$4a$	$4b$	$4c$	$8d$	$8d$	$2 \times 4a$	$2 \times 4b$	$8d$
$\cong Aem2$	c, a, b	$z, x + \frac{1}{4}, y$										$2 \times 4c$	$8d$	$2 \times 8d$

$Cmme$

No. 67

 $C2/m2/m2/e$ D_{2h}^{21}

Axes

Coordinates

Wyckoff positions

$4a$	$4b$	$4c$	$4d$	$4e$	$4f$	$4g$	$8h$	$8i$	$8j$	$8k$	$8l$
									$8m$	$8n$	$16o$

I Maximal translationengleiche subgroups[2] $C2me$ (39) $\hat{=} Aem2$ **c, -b, a** $z, -y, x$

$4a$	$4b$	$4a$	$4b$	$4c$	$4c$	$4c$	$2 \times 4a$	$2 \times 4b$	$8d$	$8d$	$8d$
									$8d$	$2 \times 4c$	$2 \times 8d$

[2] $Cm2e$ (39) $\hat{=} Aem2$ **c, a, b** $x + \frac{1}{4}, y, z$ $z, x + \frac{1}{4}, y$

$4a$	$4b$	$4c$	$4c$	$4a$	$4b$	$4c$	$8d$	$8d$	$2 \times 4a$	$2 \times 4b$	$8d$
									$2 \times 4c$	$8d$	$2 \times 8d$

 $Aem2$ C_{2v}^{15} $mm2$

Orthorhombic

No. 39

 $Aem2$ Patterson symmetry $Ammm$ ($Cmmm$)**Positions**

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

 $(0,0,0) + (0, \frac{1}{2}, \frac{1}{2}) +$

8	d	1	(1) x, y, z	(2) $\bar{x}, \bar{y}, z$	(3) $x, \bar{y} + \frac{1}{2}, z$	(4) $\bar{x}, y + \frac{1}{2}, z$
4	c	. m .	$x, \frac{1}{4}, z$	$\bar{x}, \frac{3}{4}, z$		
4	b	. . 2	$\frac{1}{2}, 0, z$	$\frac{1}{2}, \frac{1}{2}, z$		
4	a	. . 2	$0, 0, z$	$0, \frac{1}{2}, z$		

解答

Cmme

Fe 4b 222 (1/4,0,1/2)
 As 4g mm2 (0,1/4,0.654)
 O 4a 222 (1/4, 0,0)
 La 4g mm2 (0,1/4,0.145)

Aem2

Fe 4b ..2 (1/2,0,~1/4)
 As 4c .m. (0.654,3/4,~0)
 O 4a ..2 (0,0,~1/4)
 La 4c .m. (0.145,3/4,~0)

Cmme

No. 67

Axes

Coordinates

O	Fe
4a	4b

I Maximal translationengleiche subgroups

[2] C2me (39)

$\cong$ Aem2

c, -b, a

z, -y, x

4a	4b
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C2/m2/m2/e

D_{2h}^{21}

Wyckoff positions

4f	4g	8h	8i	8j	8k	8l
				8m	8n	16o

4c	2×4a	2×4b	8d	8d	8d
			8d	2×4c	2×8d

[2] C2me (39)

$\cong$ Aem2

c, -b, a

z, -y, x

No. 39

Aem2

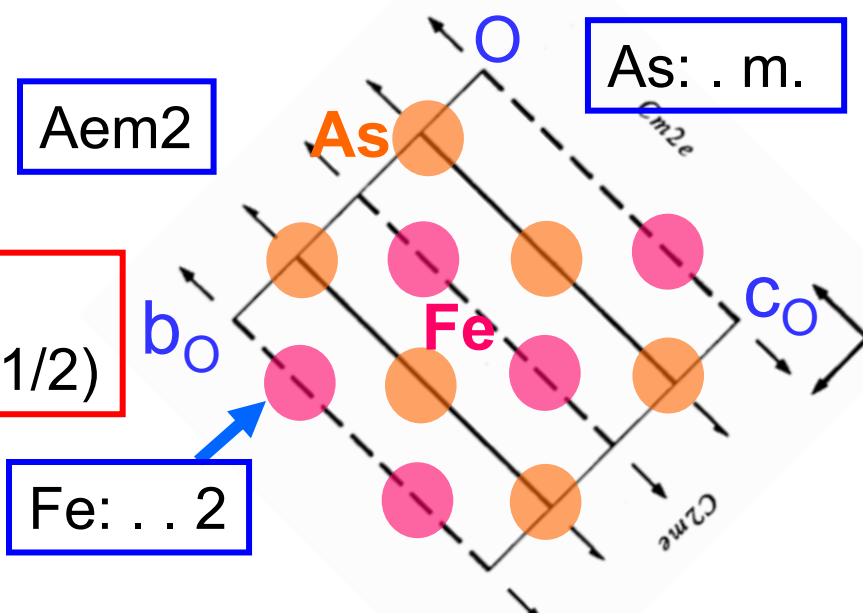
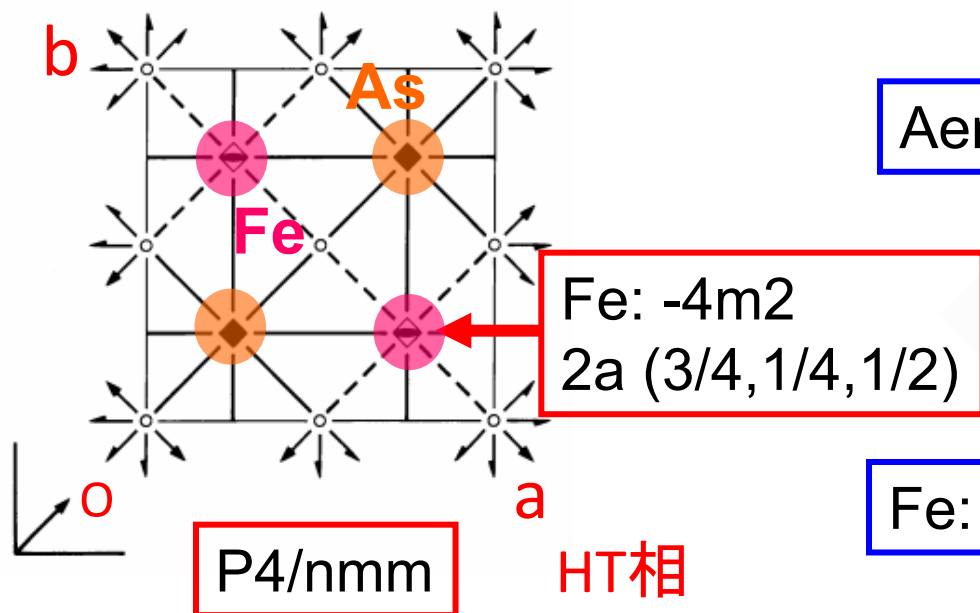
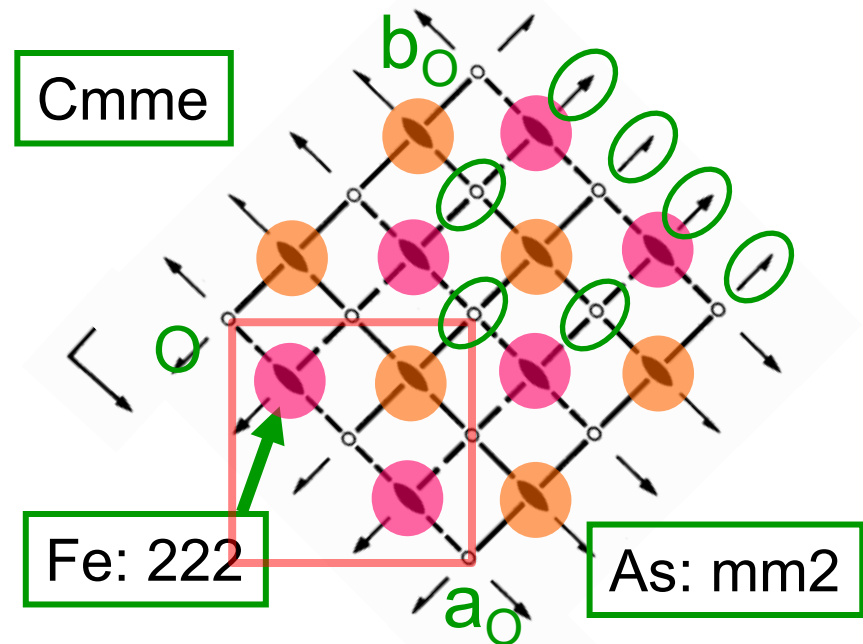
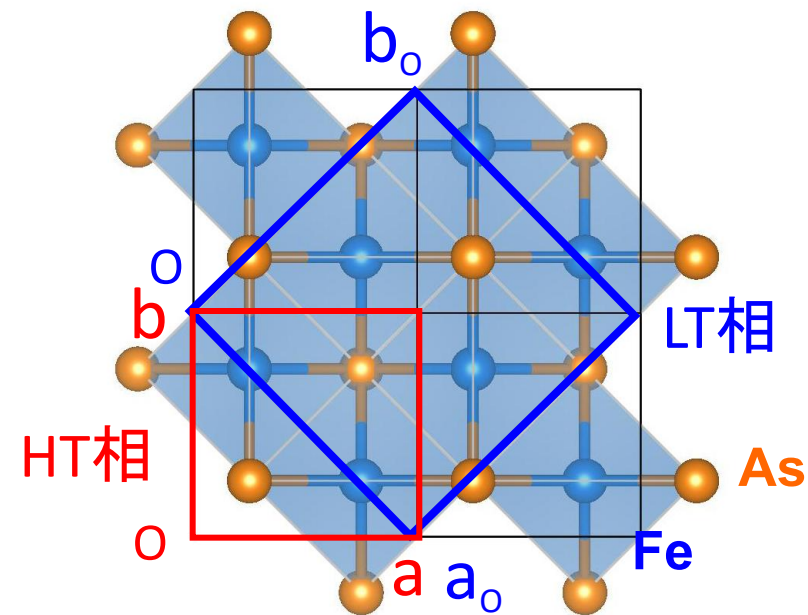
4 c . m . $x, \frac{1}{4}, z$ $\bar{x}, \frac{3}{4}, z$

4 b . . 2 $\frac{1}{2}, 0, z$ $\frac{1}{2}, \frac{1}{2}, z$

4 a . . 2 $0, 0, z$ $0, \frac{1}{2}, z$

*単位格子が(a,b,c)→(c,-b,a)に変換されている

P4/nmmからCmme, Aem2への対称性変化

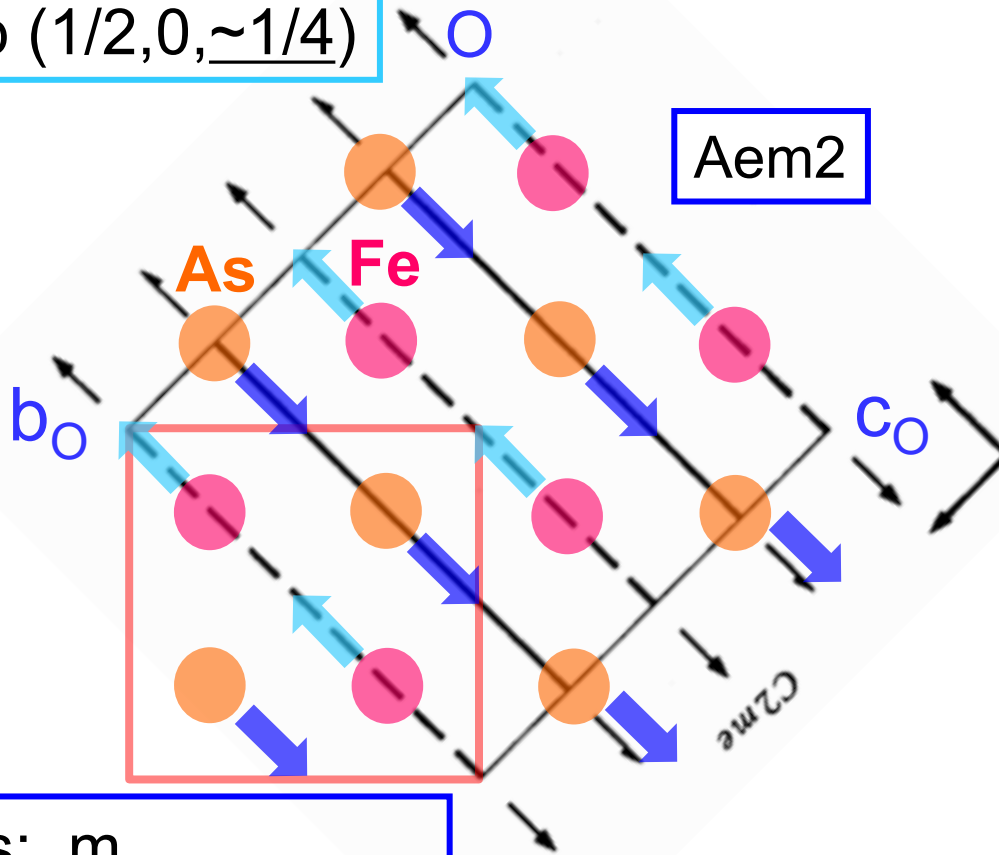


Aem2相の鉄砒素四面体の対称性

Fe: . . 2

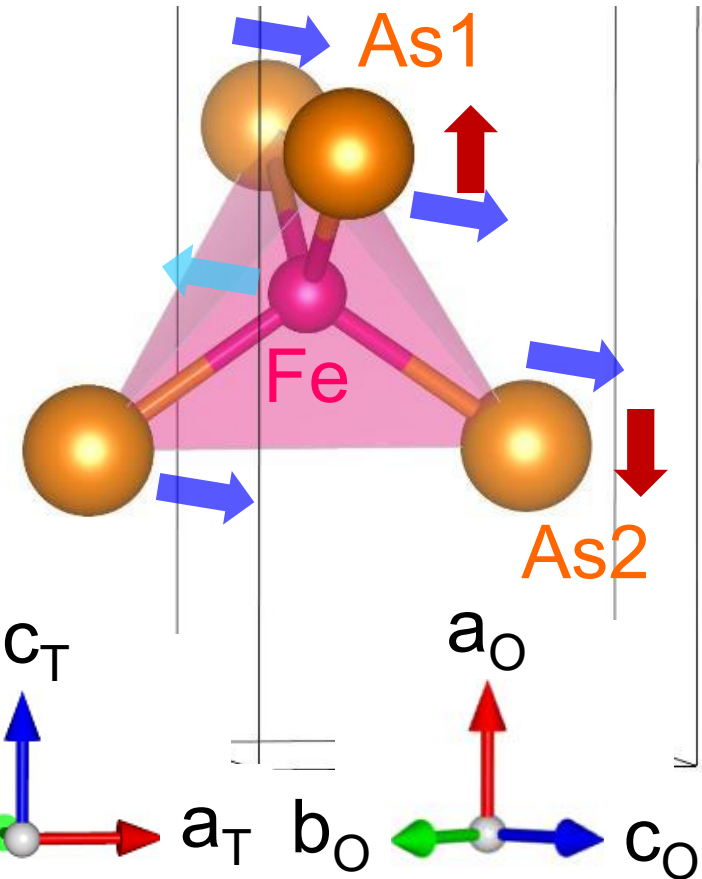
4b ($1/2, 0, \sim 1/4$)

Aem2



As: .m.

4c ($0.654, 3/4, \sim 0$)



Fe, Asの動きの制限が変化
(一方向にすべることが可能に)