Publication: lifemater.com, Author: peekAboo
Creation: 2022/3/16

弾性定数の対称性

（六方晶）

1. 六方晶の弾性定数

弾性定数C_{ijkl}について、基本的な対称性として以下の式が成立する。

$$C_{ijkl} = C_{jikl} = C_{ijlk} = C_{klij} \ . \tag{1-1}$$

直交座標におけるC_{ijkl}の座標変換を考えると、以下の式が成立する。

$$C'_{ijkl} = \sum_{m,n,p,q} C_{mnpq} l_{im} l_{jn} l_{kp} l_{lq} \ , \tag{1-2}$$

$$l_{ij} = \mathbf{e}'_i \cdot \mathbf{e}_j \ . \tag{1-3}$$

ここで、C'_{ijkl}は座標変換後の弾性定数、$\mathbf{e}'_i$は座標変換後のx'_i軸の単位ベクトル、$\mathbf{e}_i$は座標変換前のx_i軸の単位ベクトルである。

六法晶系では、直方晶系と同様に、任意のx_i軸での反転に対して対称である。そのため、Voigt 表記を用いれば、以下の式が成立する。

$$\mathbf{C} = \begin{bmatrix} C_{11} & C_{12} & C_{31} & 0 & 0 & 0 \\ C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\ C_{31} & C_{23} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{bmatrix}, \tag{1-4}$$

$$\mathbf{C}=\begin{bmatrix} C_{1111} & C_{1122} & C_{1133} & C_{1123} & C_{1131} & C_{1112} \\ C_{2211} & C_{2222} & C_{2233} & C_{2223} & C_{2231} & C_{2212} \\ C_{3311} & C_{3322} & C_{3333} & C_{3323} & C_{3331} & C_{3312} \\ C_{2311} & C_{2322} & C_{2333} & C_{2323} & C_{2331} & C_{2312} \\ C_{3111} & C_{3122} & C_{3133} & C_{3123} & C_{3131} & C_{3112} \\ C_{1211} & C_{1222} & C_{1233} & C_{1223} & C_{1231} & C_{1212} \end{bmatrix}. \tag{1-5}$$

Eq. (1-2)に代入すると、

$$C'_{ijkl}=\begin{pmatrix} \sum_{m} C_{mmmm} l_{im} l_{jm} l_{km} l_{lm} + \sum_{m,n\,(m\neq n)} C_{mmnn} l_{im} l_{jm} l_{kn} l_{ln} \\ + \sum_{m,n\,(m\neq n)} C_{mnmn} l_{im} l_{jn} l_{km} l_{ln} + \sum_{m,n\,(m\neq n)} C_{mnnm} l_{im} l_{jn} l_{kn} l_{lm} \end{pmatrix}, \tag{1-6}$$

となる。

c 軸を x_3 軸として取ると、六方晶では x_3 軸周りの 60° 回転に対して対称である。このような座標変換では、

$$l_{11}=\cos\frac{\pi}{3}=\frac{1}{2}, l_{12}=\sin\frac{\pi}{3}=\frac{\sqrt{3}}{2}, l_{21}=-\sin\frac{\pi}{3}=-\frac{\sqrt{3}}{2}, l_{22}=\cos\frac{\pi}{3}=\frac{1}{2}, l_{33}=1, \tag{1-7}$$

となるので、 $C'_{ijkl}=C_{ijkl}$ と Eq. (1-6)より、

$$\begin{aligned} C'_{1111} &= \begin{pmatrix} \sum_{m} C_{mmmm} l_{1m} l_{1m} l_{1m} l_{1m} + \sum_{m,n\,(m\neq n)} C_{mmnn} l_{1m} l_{1m} l_{1n} l_{1n} \\ + \sum_{m,n\,(m\neq n)} C_{mnmn} l_{1m} l_{1n} l_{1m} l_{1n} + \sum_{m,n\,(m\neq n)} C_{mnnm} l_{1m} l_{1n} l_{1n} l_{1m} \end{pmatrix} \\ &= \begin{pmatrix} C_{1111} l_{11} l_{11} l_{11} l_{11} + C_{2222} l_{12} l_{12} l_{12} l_{12} + 2C_{1122}\left(l_{11} l_{11} l_{12} l_{12}\right) \\ +2C_{1212}\left(l_{11} l_{12} l_{11} l_{12}\right) + 2C_{1221}\left(l_{11} l_{12} l_{12} l_{11}\right) \end{pmatrix} \\ &= C_{11} l_{11} l_{11} l_{11} l_{11} + C_{22} l_{12} l_{12} l_{12} l_{12} + 2\left(C_{12}+2C_{66}\right)\left(l_{11} l_{11} l_{12} l_{12}\right) \\ &= C_{11}\left(\frac{1}{2}\right)^4 + C_{22}\left(\frac{\sqrt{3}}{2}\right)^4 + 2\left(C_{12}+2C_{66}\right)\left(\frac{1}{2}\right)^2\left(\frac{\sqrt{3}}{2}\right)^2 \\ &= C_{11}\frac{1}{16} + C_{22}\frac{9}{16} + 2\left(C_{12}+2C_{66}\right)\frac{3}{16} = C_{11} \end{aligned},$$

$$
\begin{aligned}
C'_{2222} &= \left(\begin{aligned} &\sum_{m} C_{mmmm} l_{2m} l_{2m} l_{2m} l_{2m} + \sum_{m,n\,(m\neq n)} C_{mmnn} l_{2m} l_{2m} l_{2n} l_{2n} \\ &+ \sum_{m,n\,(m\neq n)} C_{mnmn} l_{2m} l_{2n} l_{2m} l_{2n} + \sum_{m,n\,(m\neq n)} C_{mnnm} l_{2m} l_{2n} l_{2n} l_{2m} \end{aligned} \right) \\
&= C_{1111} l_{21} l_{21} l_{21} l_{21} + C_{2222} l_{22} l_{22} l_{22} l_{22} + 2C_{1122} \left(l_{21} l_{21} l_{22} l_{22} \right) + 4C_{1212} \left(l_{21} l_{22} l_{21} l_{22} \right) \\
&= C_{11} l_{21} l_{21} l_{21} l_{21} + C_{22} l_{22} l_{22} l_{22} l_{22} + 2\left(C_{12} + 2C_{66}\right)\left(l_{21} l_{21} l_{22} l_{22} \right) , \\
&= C_{11} \left(\frac{\sqrt{3}}{2} \right)^4 + C_{22} \left(\frac{1}{2} \right)^4 + 2\left(C_{12} + 2C_{66}\right) \left(\frac{1}{2} \right)^2 \left(\frac{\sqrt{3}}{2} \right)^2 \\
&= C_{11} \frac{9}{16} + C_{22} \frac{1}{16} + 2\left(C_{12} + 2C_{66}\right) \frac{3}{16} = C_{22}
\end{aligned}
$$

となる。よって、

$$
\begin{aligned}
&C_{11} \frac{1}{16} + C_{22} \frac{9}{16} - \left(C_{11} \frac{9}{16} + C_{22} \frac{1}{16} \right) = C_{11} - C_{22} \\
&-\frac{8}{16} C_{11} + \frac{8}{16} C_{22} = C_{11} - C_{22} , \\
&-\frac{8}{16} \left(C_{11} - C_{22} \right) = C_{11} - C_{22}
\end{aligned}
$$

となるので、

$$
C_{11} = C_{22} , \tag{1-8}
$$

となる。さらに、

$$
C'_{1111} = C_{11} \frac{1}{16} + C_{22} \frac{9}{16} + 2\left(C_{12} + 2C_{66}\right) \frac{3}{16} = \frac{10}{16} C_{11} + \frac{6}{16} \left(C_{12} + 2C_{66}\right) = C_{11}
$$

$$
\begin{aligned}
&\frac{6}{16} \left(C_{12} + 2C_{66}\right) = C_{11} - \frac{10}{16} C_{11} \\
&\frac{6}{16} \left(C_{12} + 2C_{66}\right) = \frac{6}{16} C_{11} , \\
&C_{11} = C_{12} + 2C_{66}
\end{aligned}
$$

つまり、

$$
C_{66} = \frac{C_{11} - C_{12}}{2} , \tag{1-9}
$$

となる。同様にして、$C'_{ijkl} = C_{ijkl}$ と Eqs. (1-6, 1-7)より、

$$
\begin{aligned}
C'_{2233} &= \left(\begin{aligned} &\sum_{m} C_{mmmm} l_{2m} l_{2m} l_{3m} l_{3m} + \sum_{m,n\,(m\neq n)} C_{mmnn} l_{2m} l_{2m} l_{3n} l_{3n} \\ &+ \sum_{m,n\,(m\neq n)} C_{mnmn} l_{2m} l_{2n} l_{3m} l_{3n} + \sum_{m,n\,(m\neq n)} C_{mnnm} l_{2m} l_{2n} l_{3n} l_{3m} \end{aligned} \right) \\
&= \sum_{m\,(m\neq 3)} C_{mm33} l_{2m} l_{2m} l_{33} l_{33} = C_{1133} l_{21} l_{21} + C_{2233} l_{22} l_{22} \\
&= \frac{3}{4} C_{31} + \frac{1}{4} C_{23} = C_{23}
\end{aligned} ,
$$

$$
\begin{aligned}
&\frac{3}{4} C_{31} = \frac{3}{4} C_{23} , \\
&C_{31} = C_{23}
\end{aligned}
$$

となるので、

$$
C_{31} = C_{23} , \tag{1-10}
$$

が成立する。さらに、同様にして、$C'_{ijkl} = C_{ijkl}$ と Eqs. (1-6, 1-7)より、

$$
\begin{aligned}
C'_{2323} &= \left(\begin{aligned} &\sum_{m} C_{mmmm} l_{2m} l_{3m} l_{2m} l_{3m} + \sum_{m,n\,(m\neq n)} C_{mmnn} l_{2m} l_{3m} l_{2n} l_{3n} \\ &+ \sum_{m,n\,(m\neq n)} C_{mnmn} l_{2m} l_{3n} l_{2m} l_{3n} + \sum_{m,n\,(m\neq n)} C_{mnnm} l_{2m} l_{3n} l_{2n} l_{3m} \end{aligned} \right) \\
&= \sum_{m\,(m\neq 3)} C_{m3m3} l_{2m} l_{33} l_{2m} l_{33} = C_{1313} l_{21} l_{21} + C_{2323} l_{22} l_{22} \\
&= \frac{1}{4} C_{55} + \frac{3}{4} C_{44} = C_{44}
\end{aligned} ,
$$

$$
\begin{aligned}
&\frac{1}{4} C_{55} = \frac{1}{4} C_{44} , \\
&C_{55} = C_{44}
\end{aligned}
$$

となるので、

$$
C_{55} = C_{44} , \tag{1-11}
$$

が成立する。なお、

$$
\begin{aligned}
C'_{1122} &= \begin{pmatrix} \sum_{m} C_{mmmm} l_{1m} l_{1m} l_{2m} l_{2m} + \sum_{m,n\,(m\neq n)} C_{mmnn} l_{1m} l_{1m} l_{2n} l_{2n} \\ + \sum_{m,n\,(m\neq n)} C_{mnmn} l_{1m} l_{1n} l_{2m} l_{2n} + \sum_{m,n\,(m\neq n)} C_{mnnm} l_{1m} l_{1n} l_{2n} l_{2m} \end{pmatrix} \\
&= \begin{pmatrix} C_{1111} l_{11} l_{11} l_{21} l_{21} + C_{2222} l_{12} l_{12} l_{22} l_{22} + C_{1122} \left(l_{11} l_{11} l_{22} l_{22} + l_{12} l_{12} l_{21} l_{21} \right) \\ + C_{1212} \left(l_{11} l_{12} l_{21} l_{22} + l_{12} l_{11} l_{22} l_{21} + l_{11} l_{12} l_{22} l_{21} + l_{12} l_{11} l_{21} l_{22} \right) \end{pmatrix} \\
&= C_{11} l_{11} l_{11} l_{21} l_{21} + C_{22} l_{12} l_{12} l_{22} l_{22} + C_{12} \left(l_{11} l_{11} l_{22} l_{22} + l_{12} l_{12} l_{21} l_{21} \right) + 4C_{66} l_{11} l_{12} l_{21} l_{22} \\
&= C_{11} \left(\frac{1}{2}\right)^2 \left(\frac{\sqrt{3}}{2}\right)^2 + C_{22} \left(\frac{1}{2}\right)^2 \left(\frac{\sqrt{3}}{2}\right)^2 + C_{12} \left(\left(\frac{1}{2}\right)^4 + \left(\frac{\sqrt{3}}{2}\right)^4 \right) - 4C_{66} \left(\frac{1}{2}\right)^2 \left(\frac{\sqrt{3}}{2}\right)^2 \\
&= \frac{6}{16} C_{11} + \frac{10}{16} C_{12} - \frac{12}{16} C_{66} = \frac{6}{16} \left(C_{12} + 2C_{66} \right) + \frac{10}{16} C_{12} - \frac{12}{16} C_{66} \\
&= \frac{6}{16} C_{12} + \frac{12}{16} C_{66} + \frac{10}{16} C_{12} - \frac{12}{16} C_{66} = C_{12}
\end{aligned}
$$

となっている。

よって、Eqs. (1-8~1-11)より、

$$
\mathbf{C} = \begin{bmatrix} C_{11} & C_{12} & C_{23} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{23} & 0 & 0 & 0 \\ C_{23} & C_{23} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \dfrac{C_{11} - C_{12}}{2} \end{bmatrix}, \qquad (1\text{-}12)
$$

となる。