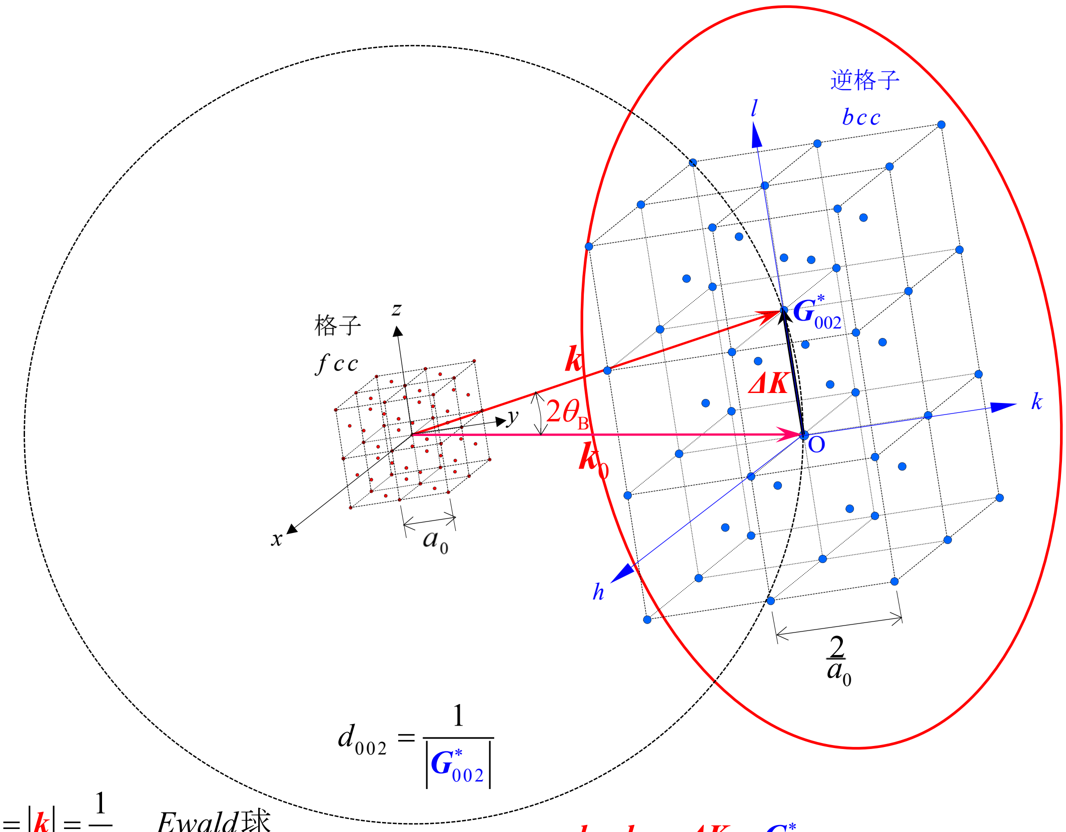


$|k_0| = |k| = \frac{1}{\lambda}$　　*Ewald*球

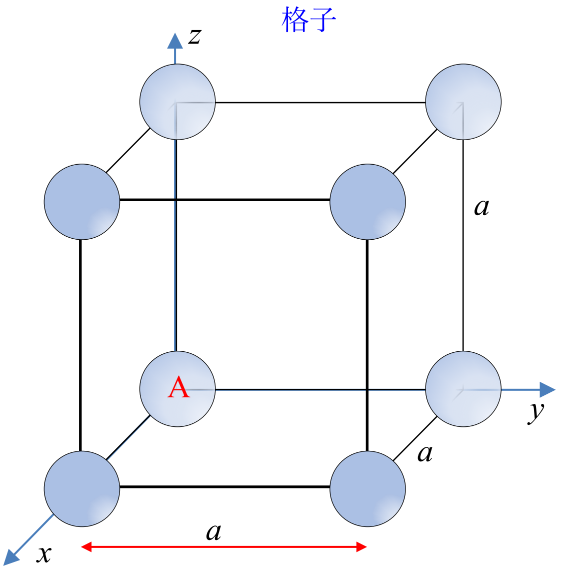
$k - k_0 = \Delta K = G^*_{002}$

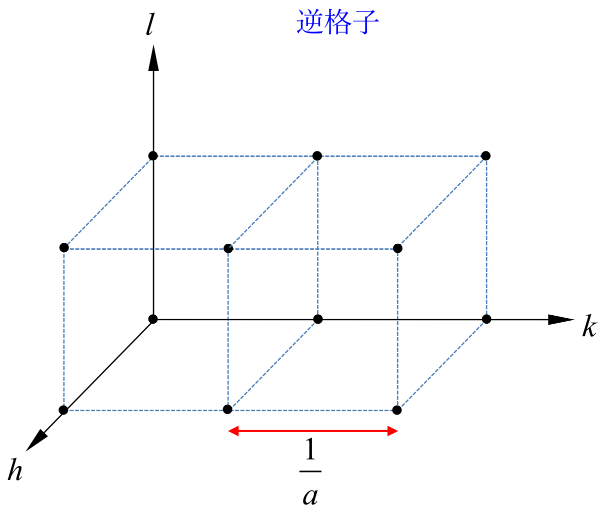
§　結晶構造因子の計算例

$$F(h,\,k,\,l)=\sum_{j=1}^{\text{単位胞}} f_j(\frac{\sin\theta}{\lambda})\,e^{2\pi i(hx_j+ky_j+lz_j)} \qquad (1)$$

hkl	ミラー指数　→　逆格子点　⇔　(hkl)面
$x_j,\,y_j,\,z_j$	単位胞内の原子座標（格子定数＝1としている）
f_j	原子散乱因子（j原子の電子密度分布の Fourier 変換 (X 線)）
F	結晶構造因子（単位胞の Fourier 変換）

1. 単純立方格子





a_0^3 中に 1 個の原子　その座標は a_0 を単位として $\begin{pmatrix}x\\y\\z\end{pmatrix}=\overset{\text{A}}{\begin{pmatrix}0\\0\\0\end{pmatrix}}$

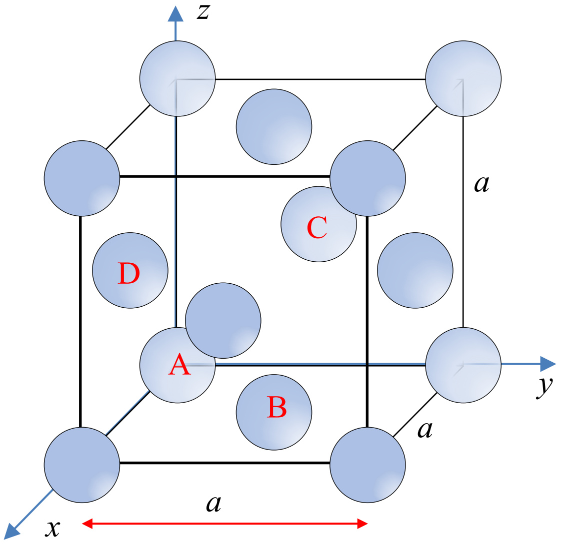
$$\therefore\quad F(h,k,l)=f\,e^{2\pi i(h\times0+k\times0+l\times0)}=f\,e^{2\pi i\times0}=f\,e^{0}=f$$ for all h,k,l（すべての h,k,l に対して）

ちなみに $\frac{1}{8}$ 個の原子が $\begin{pmatrix}0\\0\\0\end{pmatrix},\begin{pmatrix}1\\0\\0\end{pmatrix},\begin{pmatrix}0\\1\\0\end{pmatrix},\begin{pmatrix}0\\0\\1\end{pmatrix},\begin{pmatrix}1\\1\\0\end{pmatrix},\begin{pmatrix}1\\0\\1\end{pmatrix},\begin{pmatrix}0\\1\\1\end{pmatrix},\begin{pmatrix}1\\1\\1\end{pmatrix}$ にあるとすると、

$$F(h,k,l)=\frac{f}{8}\left\{e^{2\pi i(h\times0+k\times0+l\times0)}+e^{2\pi ih}+e^{2\pi ik}+e^{2\pi il}+e^{2\pi i(h+k)}+e^{2\pi i(k+l)}+e^{2\pi i(l+h)}+e^{2\pi i(h+k+l)}\right\}$$

$$=\frac{f}{8}\{1+1+1+1+1+1+1+1\}=f$$ 結果は同じになる

2. 面心立方格子



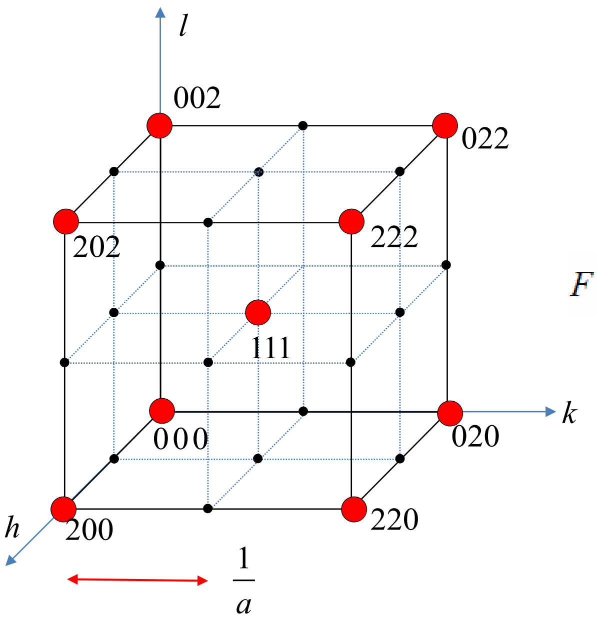
$$
a^3 \text{ 中に 4 個の原子　その座標は } a \text{ を単位として }
\begin{array}{c}
 \\
\begin{pmatrix} x \\ y \\ z \end{pmatrix} =
\end{array}
\begin{array}{cccc}
\mathrm{A} & \mathrm{B} & \mathrm{C} & \mathrm{D} \\
\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, & \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix}, & \begin{pmatrix} 0 \\ 1/2 \\ 1/2 \end{pmatrix}, & \begin{pmatrix} 1/2 \\ 0 \\ 1/2 \end{pmatrix}
\end{array}
$$

$$
\therefore \quad F(h,k,l) = f\left\{ e^{2\pi i\times 0} + e^{\pi i(h+k)} + e^{\pi i(k+l)} + e^{\pi i(h+l)} \right\}
$$

$$
\downarrow \leftarrow \quad e^{\pi i n} = \cos n\pi + i\sin n\pi = \cos n\pi + 0 = (-1)^n
$$

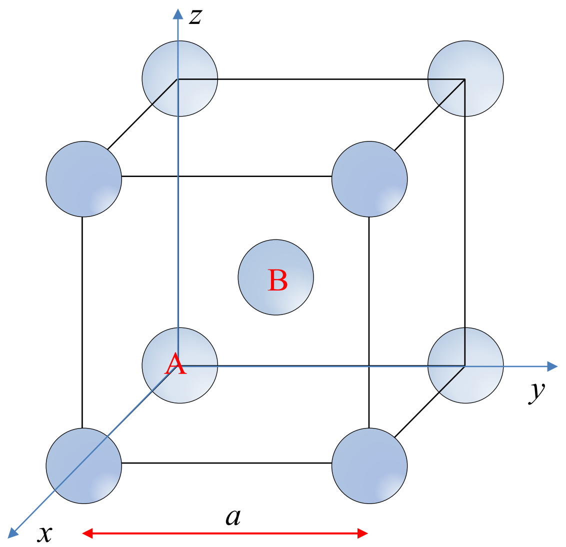
$$
= f\left\{ 1 + (-1)^{h+k} + (-1)^{k+l} + (-1)^{l+h} \right\}
$$

$$
= \begin{cases} 4f & for\ \ h,k,l = all\, even\ \ or\ \ all\, odd \\ 0 & for\ \ h,k,l = even, odd\ \ mixed \end{cases}
$$



$$
F(h,k,l) = \begin{cases} 4f & for\ \ h,k,l = all\, even\ \ or\ \ all\, odd \\ 0 & for\ \ h,k,l = even, odd\ \ mixed \end{cases}
$$

3. 体心立方格子



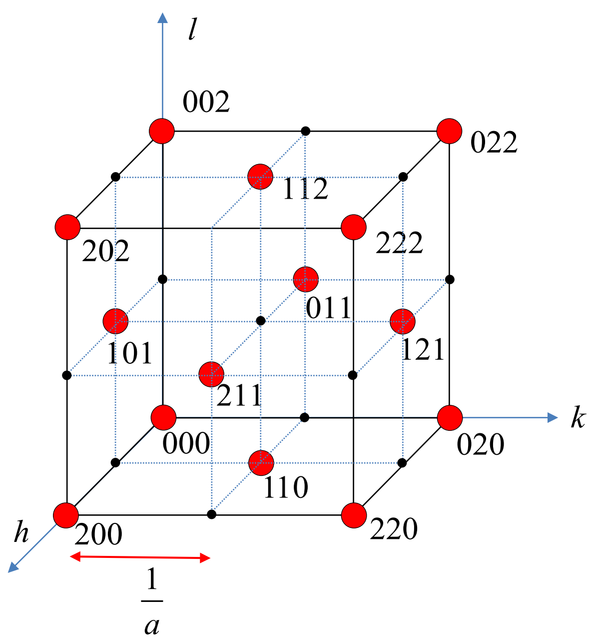
a_0^3 中に 2 個の原子　その座標は a_0 を単位として

$$\begin{array}{ccc} & \text{A} & \text{B} \\ \begin{pmatrix} x \\ y \\ z \end{pmatrix} = & \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, & \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix} \end{array}$$

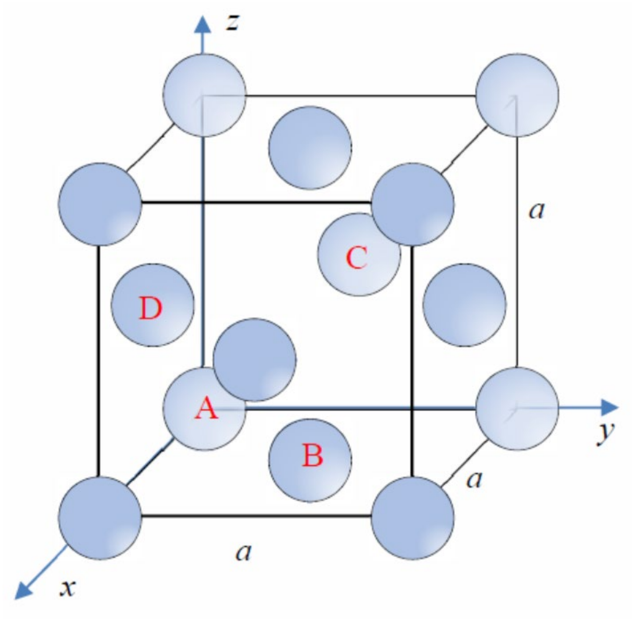
$$F(h,k,l) = f\left\{ e^{2\pi i(h\times 0 + k\times 0 + l\times 0)} + e^{2\pi i\left(\frac{h}{2}+\frac{k}{2}+\frac{l}{2}\right)} \right\}$$

$$\therefore \quad = f\left\{1 + (-1)^{h+k+l}\right\}$$

$$= \begin{cases} 2f & for\ h+k+l = even \\ 0 & for\ h+k+l = odd \end{cases}$$



$$F(h,k,l) = \begin{cases} 2f & for\ h+k+l = even \\ 0 & for\ h+k+l = odd \end{cases}$$


z
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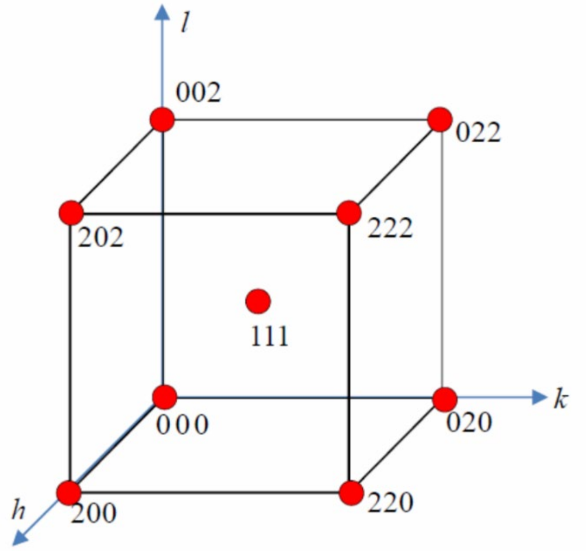
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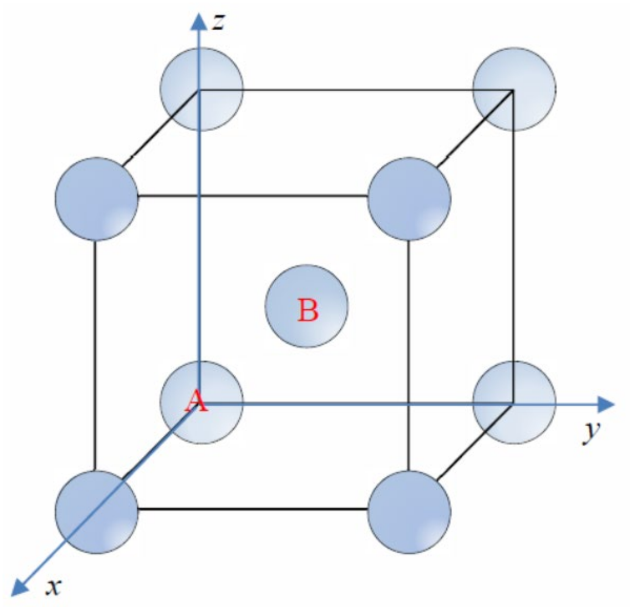
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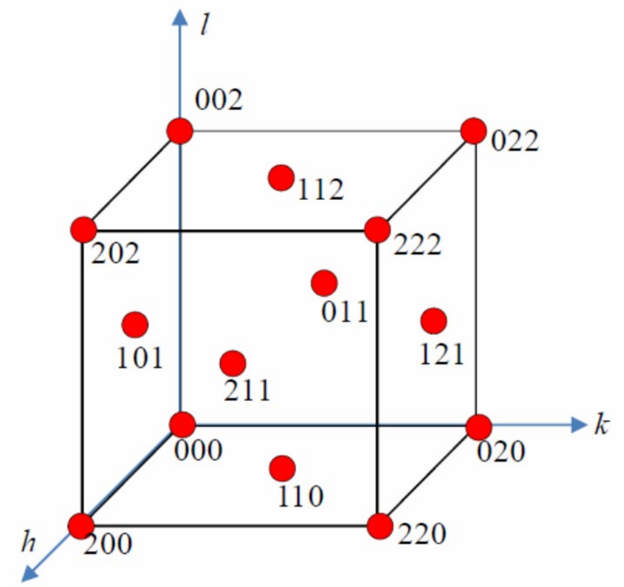
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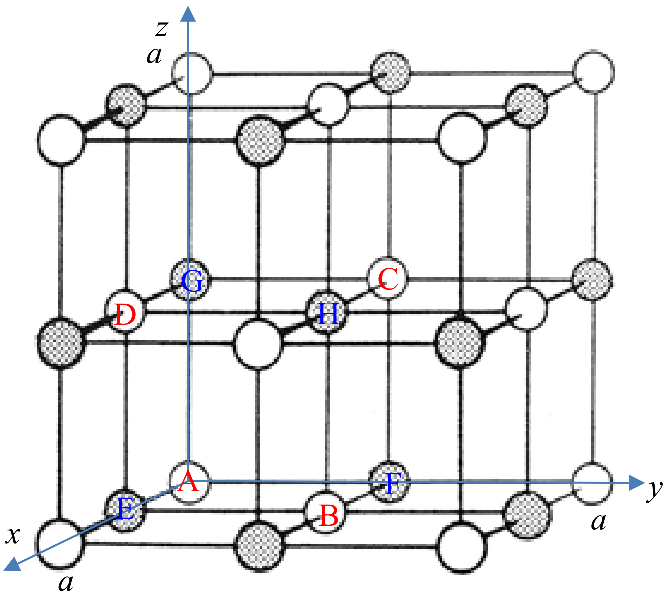
4. 食塩型格子



a^3 中に A 原子 4 個、B 原子 4 個　その座標は a を単位として

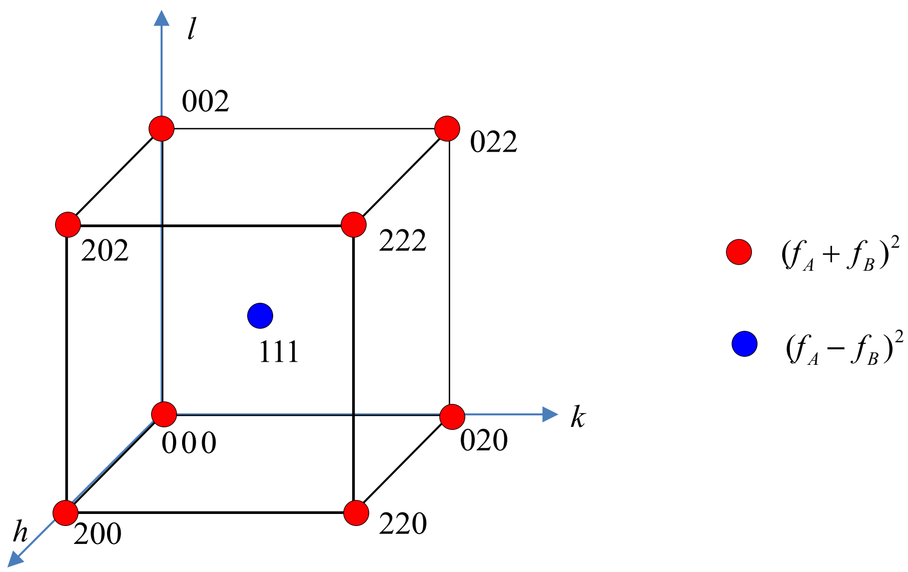
A 原子: $\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \overset{A}{\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}}, \overset{B}{\begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix}}, \overset{C}{\begin{pmatrix} 0 \\ 1/2 \\ 1/2 \end{pmatrix}}, \overset{D}{\begin{pmatrix} 1/2 \\ 0 \\ 1/2 \end{pmatrix}}$　　B 原子: $\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \overset{E}{\begin{pmatrix} 1/2 \\ 0 \\ 0 \end{pmatrix}}, \overset{F}{\begin{pmatrix} 0 \\ 1/2 \\ 0 \end{pmatrix}}, \overset{G}{\begin{pmatrix} 0 \\ 0 \\ 1/2 \end{pmatrix}}, \overset{H}{\begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix}}$

$$F(h,k,l) = f_A\left\{e^{2\pi i(h\times 0+k\times 0+l\times 0)} + e^{2\pi i\left(\frac{h}{2}+\frac{k}{2}\right)} + e^{2\pi i\left(\frac{k}{2}+\frac{l}{2}\right)} + e^{2\pi i\left(\frac{l}{2}+\frac{h}{2}\right)}\right\} + f_B\left\{e^{2\pi i\frac{h}{2}} + e^{2\pi i\frac{k}{2}} + e^{2\pi i\frac{l}{2}} + e^{2\pi i\left(\frac{h}{2}+\frac{k}{2}+\frac{l}{2}\right)}\right\}$$

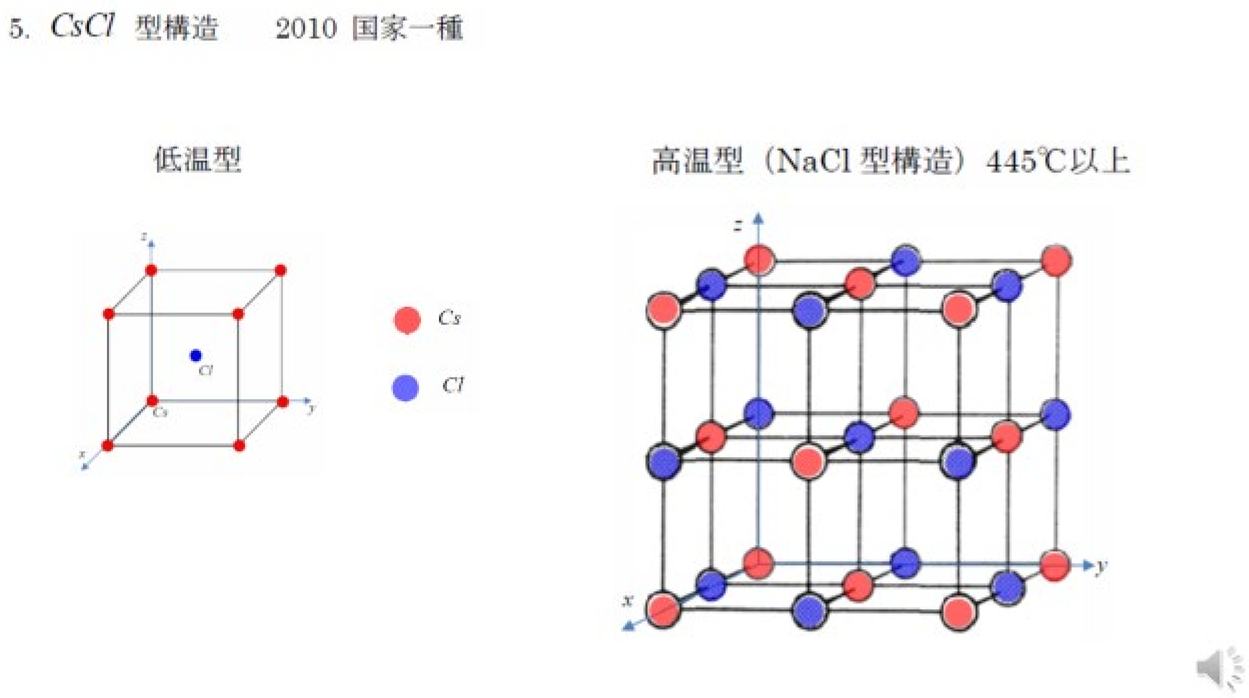
$$= f_A\left\{1 + e^{\pi i(h+k)} + e^{\pi i(k+l)} + e^{\pi i(l+h)}\right\} + f_B\left\{e^{\pi i h} + e^{\pi i k} + e^{\pi i l} + e^{\pi i(h+k+l)}\right\}$$

$$= f_A\left\{1 + (-1)^{h+k} + (-1)^{k+l} + (-1)^{l+h}\right\} + f_B(-1)^{h+k+l}\left\{(-1)^{k+l} + (-1)^{l+h} + (-1)^{h+k} + 1\right\}$$

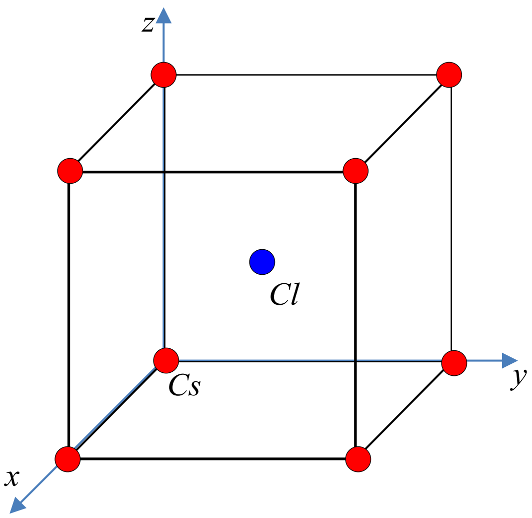
$$= \boxed{\begin{gathered}(f_A + (-1)^{h+k+l} f_B) \\ = \begin{cases} f_A + f_B & \text{for } h+k+l = even \\ f_A - f_B & \text{for } h+k+l = odd \end{cases}\end{gathered}} \times \boxed{\begin{gathered}\left\{1 + (-1)^{h+k} + (-1)^{k+l} + (-1)^{l+h}\right\} \\ = \begin{cases} 4 & \text{for } hkl \text{ all even or all odd} \\ 0 & \text{for mixed } hkl \end{cases}\end{gathered}}$$



5. $CsCl$ 型構造　　2010 国家一種



低温型

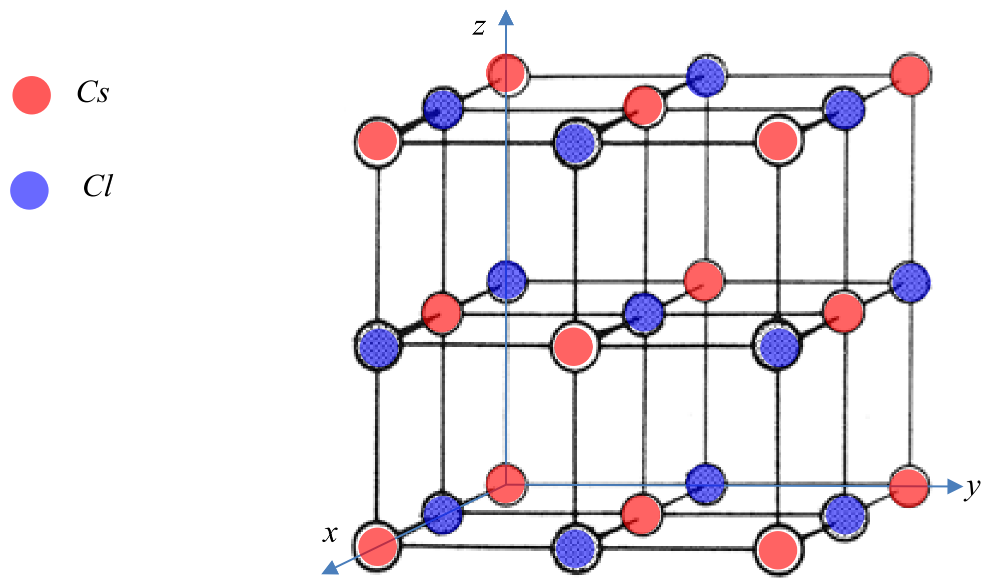


単純立方格子

a^3 中に Cs$^+$イオン 1 個 $\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$、Cl$^-$イオン $\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix}$

$$F(h,k,l) = f_{Cs}\, e^{2\pi i(h\times 0 + k\times 0 + l\times 0)} + f_{Cl} e^{2\pi i\left(\frac{h}{2}+\frac{k}{2}+\frac{l}{2}\right)} = f_{Cs} + f_{Cl}(-1)^{h+k+l} = \begin{cases} f_{Cs} + f_{Cl} & for\ \ h,k,l\ \ all\ even \\ f_{Cs} - f_{Cl} & for\ \ h,k,l\ \ 2\text{つ}even\ 1\text{つ}odd \\ f_{Cs} + f_{Cl} & for\ \ h,k,l\ \ 1\text{つ}even\ 2\text{つ}odd \\ f_{Cs} - f_{Cl} & for\ \ h,k,l\ \ all\ odd \end{cases}$$

高温型（NaCl 型構造）445℃以上

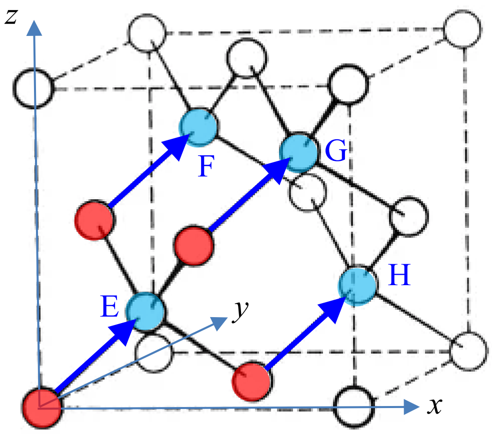


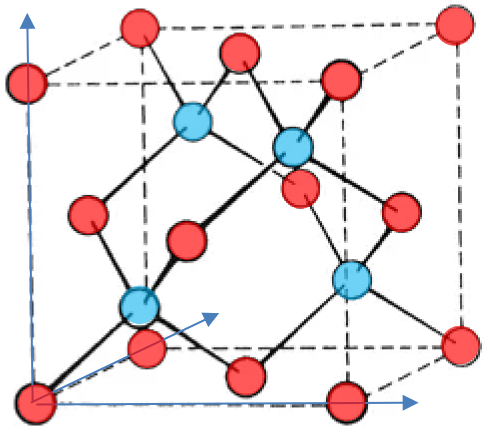
$$F(h,k,l) = \begin{cases} 4(f_{Cs} + f_{Cl}) & for\ \ h,k,l\ \ all\ even \\ 0 & for\ \ h,k,l\ \ 2\text{つ}even\ 1\text{つ}odd \\ 0 & for\ \ h,k,l\ \ 1\text{つ}even\ 2\text{つ}odd \\ 4(f_{Cs} - f_{Cl}) & for\ \ h,k,l\ \ all\ odd \end{cases}$$

6. 閃亜鉛鉱型構造　(Zinc-blend type of structure)

Ga 原子: $\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1/2 \\ 1/2 \end{pmatrix}, \begin{pmatrix} 1/2 \\ 0 \\ 1/2 \end{pmatrix}, \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix}$

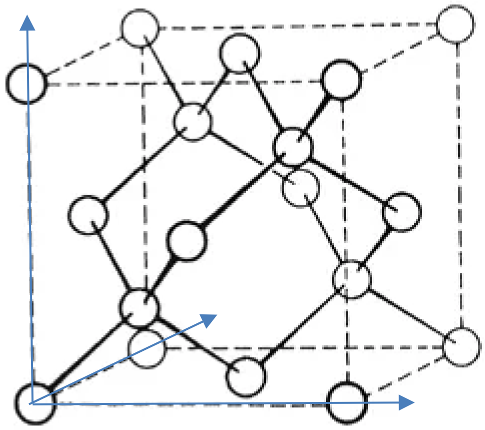
As 原子: $\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{array}{cccc} \text{E} & \text{F} & \text{G} & \text{H} \\ \begin{pmatrix} 1/4 \\ 1/4 \\ 1/4 \end{pmatrix}, & \begin{pmatrix} 1/4 \\ 3/4 \\ 3/4 \end{pmatrix}, & \begin{pmatrix} 3/4 \\ 1/4 \\ 3/4 \end{pmatrix}, & \begin{pmatrix} 3/4 \\ 3/4 \\ 1/4 \end{pmatrix} \end{array}$





7. ダイヤモンド型構造

C 原子: $\begin{pmatrix}x\\y\\z\end{pmatrix}=\begin{pmatrix}0\\0\\0\end{pmatrix},\begin{pmatrix}1/2\\1/2\\0\end{pmatrix},\begin{pmatrix}1/2\\0\\1/2\end{pmatrix},\begin{pmatrix}0\\1/2\\1/2\end{pmatrix},\begin{pmatrix}1/4\\1/4\\1/4\end{pmatrix},\begin{pmatrix}3/4\\3/4\\1/4\end{pmatrix},\begin{pmatrix}3/4\\1/4\\3/4\end{pmatrix},\begin{pmatrix}1/4\\3/4\\3/4\end{pmatrix}$



$$
\begin{aligned}
F/f &= e^{2\pi i(0+0+0)}+e^{2\pi i\left(\frac{h}{2}+\frac{k}{2}+0\right)}+e^{2\pi i\left(\frac{h}{2}+0+\frac{l}{2}\right)}+e^{2\pi i\left(0+\frac{k}{2}+\frac{l}{2}\right)}+e^{2\pi i\left(\frac{h}{4}+\frac{k}{4}+\frac{l}{4}\right)}+e^{2\pi i\left(\frac{3h}{4}+\frac{3k}{4}+\frac{l}{4}\right)}+e^{2\pi i\left(\frac{3h}{4}+\frac{k}{4}+\frac{3l}{4}\right)}+e^{2\pi i\left(\frac{h}{4}+\frac{3k}{4}+\frac{3l}{4}\right)}\\
&=1+e^{\pi i(h+k)}+e^{\pi i(h+l)}+e^{\pi i(k+l)}+e^{\pi i\left(\frac{h+k+l}{2}\right)}+e^{\pi i\left(\frac{3h+3k+l}{2}\right)}+e^{\pi i\left(\frac{3h+k+3l}{2}\right)}+e^{\pi i\left(\frac{h+3k+3l}{2}\right)}\\
&=\left(1+e^{\pi i(h+k)}+e^{\pi i(h+l)}+e^{\pi i(k+l)}\right)+e^{\pi i\left(\frac{h+k+l}{2}\right)}\left(1+e^{\pi i(h+k)}+e^{\pi i(h+l)}+e^{\pi i(k+l)}\right)\\
&=\left(1+e^{\pi i\left(\frac{h+k+l}{2}\right)}\right)\left(1+e^{\pi i(h+k)}+e^{\pi i(h+l)}+e^{\pi i(k+l)}\right)\\
&=\left(1+e^{\pi i\left(\frac{h+k+l}{2}\right)}\right)\left(1+(-1)^{(h+k)}+(-1)^{(h+l)}+(-1)^{(k+l)}\right)
\end{aligned}
$$

$$
\downarrow\leftarrow\left(1+(-1)^{(h+k)}+(-1)^{(h+l)}+(-1)^{(k+l)}\right)=\begin{cases}4 & hkl\ all\ even\\ 4 & hkl\ all\ odd\\ 0 & hkl\ even\ odd\ mix\end{cases}
$$

さらに　hkl　$all\ even$　または $all\ odd$ の場合

$$
F/f=4\left(1+e^{\pi i\left(\frac{h+k+l}{2}\right)}\right)
$$

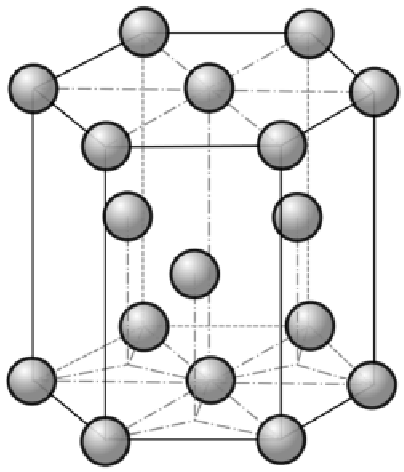
よって

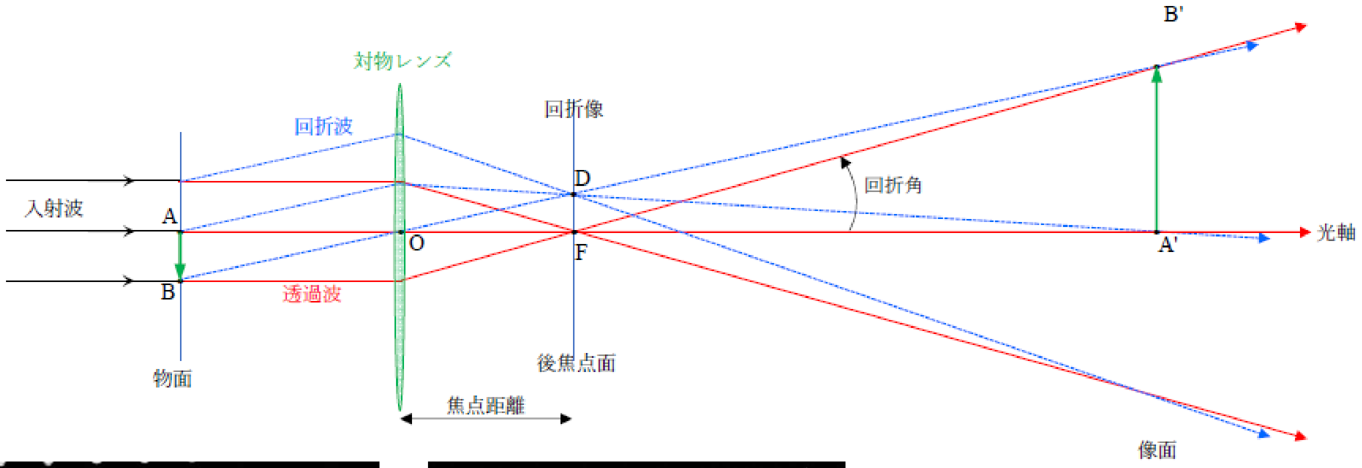
$$
|F|^2=16f^2\left(1+e^{\pi i\left(\frac{h+k+l}{2}\right)}\right)\left(1+e^{-\pi i\left(\frac{h+k+l}{2}\right)}\right)=|F|^2=16f^2\left(2+2\cos\frac{\pi}{2}(h+k+l)\right)
$$

$$
=32f^2\left(1+\cos\frac{\pi}{2}(h+k+l)\right)=32f^2\times\begin{cases}2 & for\ h+k+l=4n\\ 1 & for\ h+k+l=4n+1\\ 0 & for\ h+k+l=4n+2\\ 1 & for\ h+k+l=4n+3\end{cases}
$$

8. hcp Co

$$\begin{pmatrix} a_1 \\ a_2 \\ c \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 2/3 \\ 1/3 \\ 1/2 \end{pmatrix}$$




B'
対物レンズ
回折像
回折波
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回折角
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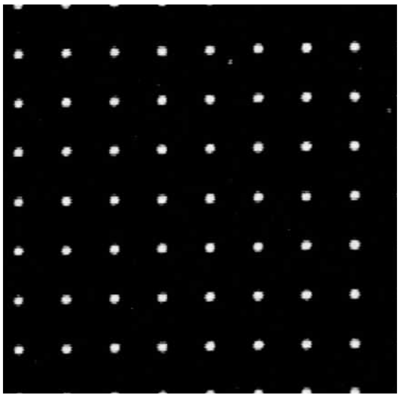
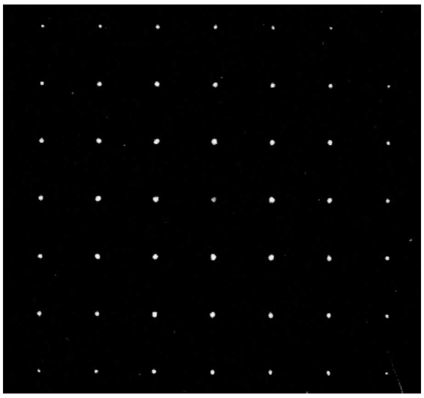
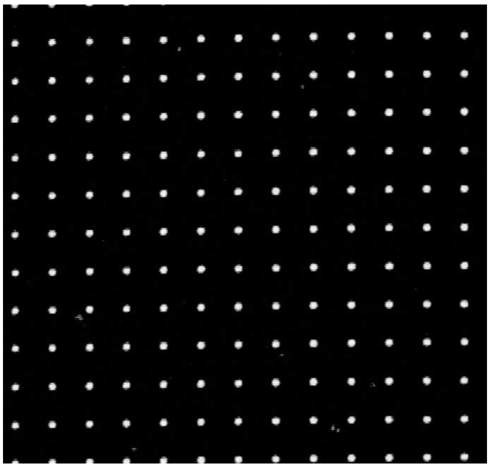
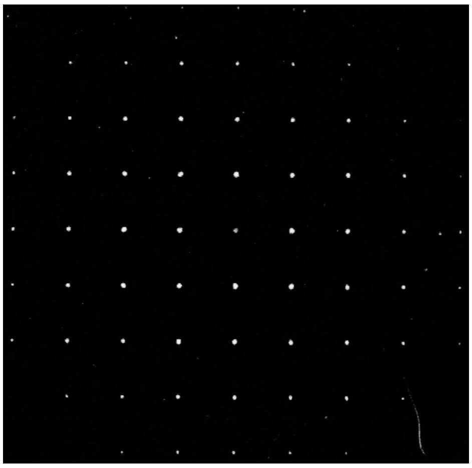
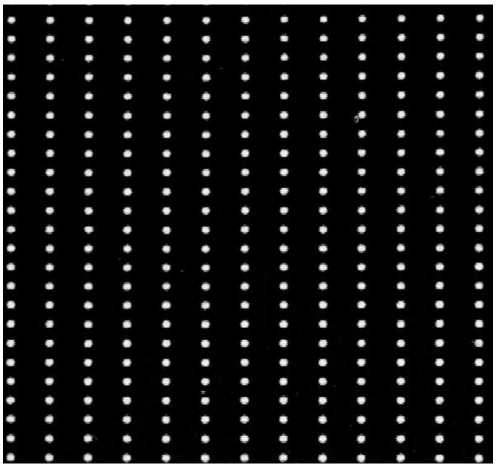
後焦点面
物面
焦点距離
像面

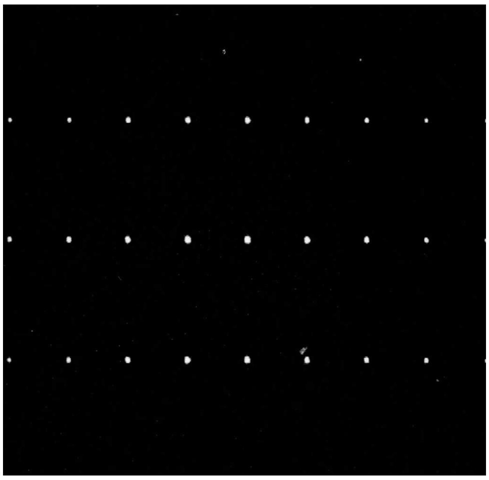


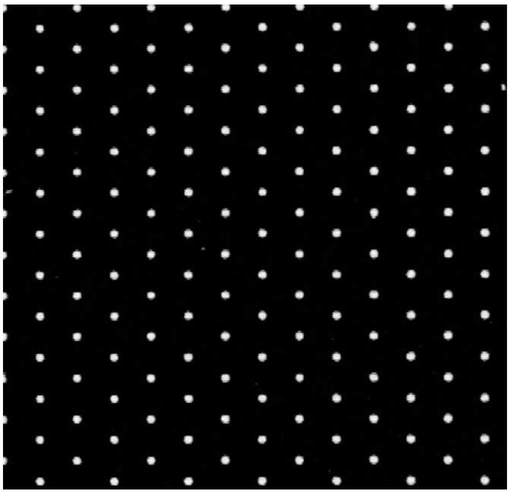


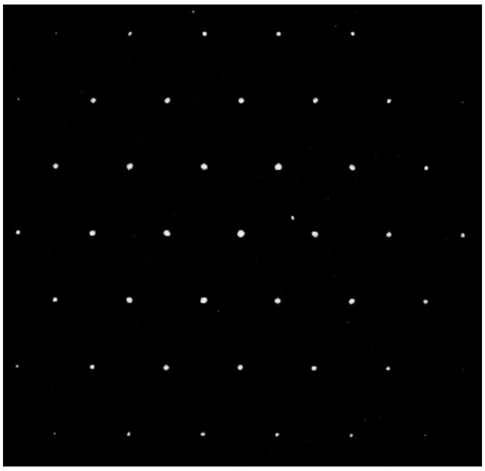


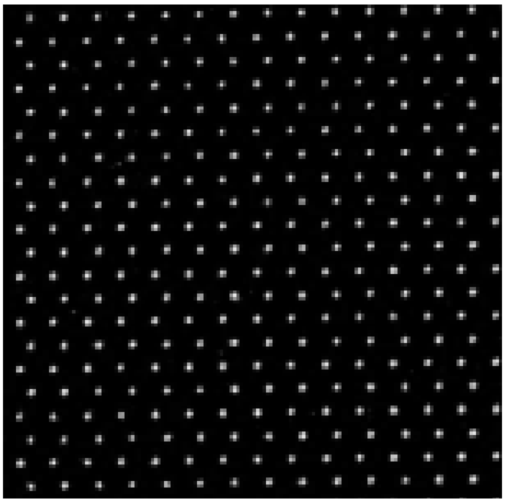


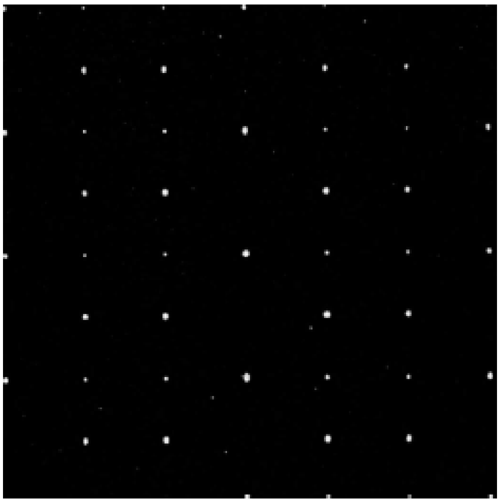


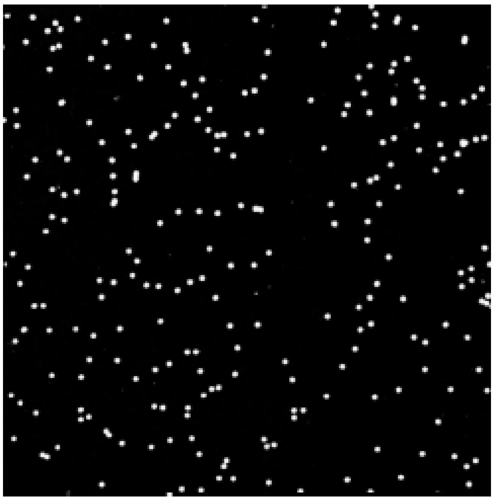
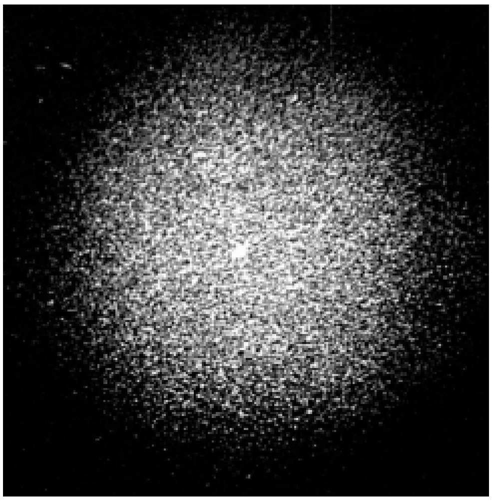


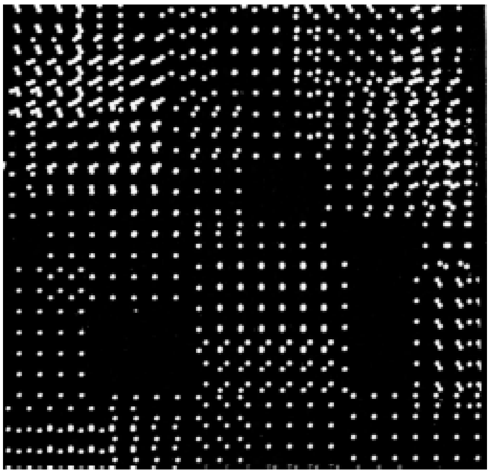
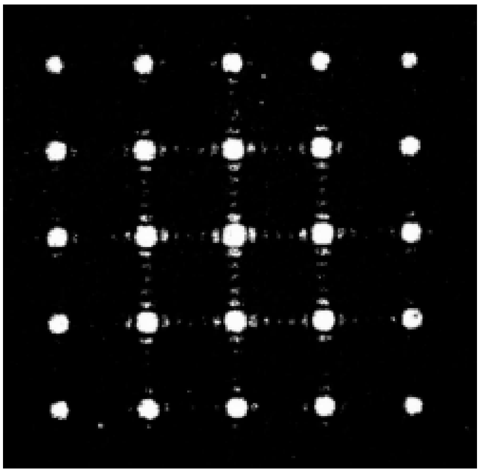


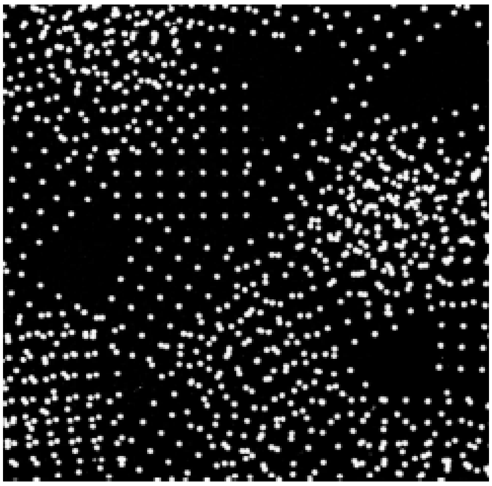
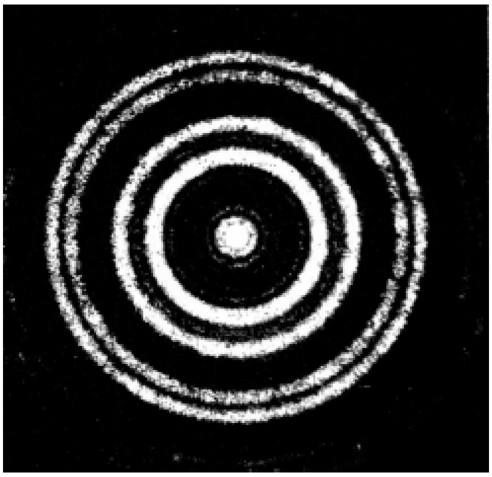


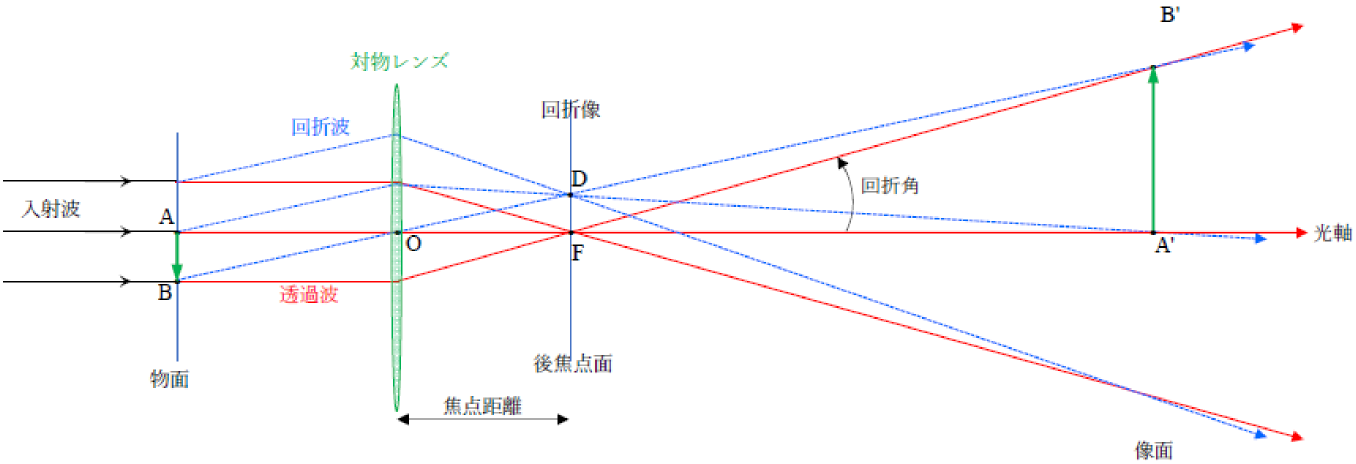





B'
対物レンズ
回折像
回折波
D
回折角
入射波
A
O
F
光軸
A'
B
透過波
後焦点面
物面
焦点距離
像面