Acta Cryst A
FOUNDATIONS ADVANCES

ISSN 2053-2733

Received 17 April 2019
Accepted 8 May 2019

Edited by K. Tsuda, Tohoku University, Japan

Keywords: diffraction moiré fringes; *Pendellösung* oscillation; phase jump; gap phase.

Theoretical study of the properties of X-ray diffraction moiré fringes. I. Corrigenda and addenda

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Seven corrections are made and several supplementary equations are added to the article by Yoshimura [*Acta Cryst.* (2015), A**71**, 368–381].

On p. 371, left column, near the top, just after 'the index (i) = (1, 2) ... dispersion surface', the following comment should be added: 'the upper sine in equations (5a), (5b) refers to the case of $i = 1$, and the lower sine to the case of $i = 2$'. On p. 371, right column, near the bottom, just after 'the indices (i, j) = (1, 2) ..., respectively', the following comment should be added: 'the upper sign in equations (15a) to (15d) refers to the case of $j = 1$, and the lower sine to the case of $j = 2$'. Equations (14b), (14c) are incorrect. They must be corrected to

$$\begin{aligned} E^{i,j}_{og'}(\mathbf{r}) &= C^i_o C^{i,j}_{og'} \exp 2\pi i(\mathbf{g}' \cdot \mathbf{r}_b) \exp i\big\{(\mathbf{K}_e \cdot \mathbf{r}_a) + [\mathbf{k}^i_o \cdot (\mathbf{r}_{a'} - \mathbf{r}_a)] \\ &\quad + [\mathbf{K}^i_o \cdot (\mathbf{r}_b - \mathbf{r}_{a'})] + [\mathbf{k}^{i,j}_{og'} \cdot (\mathbf{r}_{b'} - \mathbf{r}_b)] \\ &\quad + [\mathbf{K}^{i,j}_{og'} \cdot (\mathbf{r} - \mathbf{r}_{b'})]\big\} \\ &= C^i_o C^{i,j}_{og'} \exp i\big[-K\delta^i_a t_1 - K\delta^{i,j}_{b,oo'} t_2 + u_n T_{b'}/\gamma_g \\ &\quad - 2\pi(\Delta\mathbf{g} \cdot \hat{\mathbf{K}}_g) T_{b'}/\gamma_g\big] \exp i[(\mathbf{K}_e + 2\pi\mathbf{g}') \cdot \mathbf{r}], \end{aligned} \tag{14b}$$

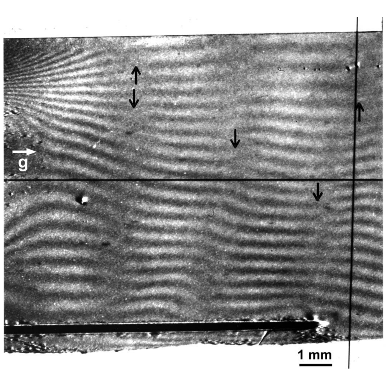
$$\begin{aligned} E^{i,j}_{go'}(\mathbf{r}) &= C^i_g C^{i,j}_{go'} \exp 2\pi i[(\mathbf{g} \cdot \mathbf{r}_a) - (\mathbf{g}' \cdot \mathbf{r}_b)] \exp i\big\{(\mathbf{K}_e \cdot \mathbf{r}_a) \\ &\quad + [\mathbf{k}^i_g \cdot (\mathbf{r}_{a'} - \mathbf{r}_a)] + [\mathbf{K}^i_g \cdot (\mathbf{r}_b - \mathbf{r}_{a'})] + [\mathbf{k}^{i,j}_{go'} \cdot (\mathbf{r}_{b'} - \mathbf{r}_b)] \\ &\quad + [\mathbf{K}^{i,j}_{go'} \cdot (\mathbf{r} - \mathbf{r}_{b'})]\big\} \\ &= C^i_g C^{i,j}_{go'} \exp i\big[-K\delta^i_a t_1 - K\delta^{i,j}_{b,gg'} t_2 + u_n (T_{a'} - T_{b'})/\gamma_g \\ &\quad + 2\pi(\Delta\mathbf{g} \cdot \hat{\mathbf{K}}_o) T_{b'}/\gamma_o\big] \exp i[(\mathbf{K}_e - 2\pi\Delta\mathbf{g}) \cdot \mathbf{r}]. \end{aligned} \tag{14c}$$

In these corrections, the last terms in the first exponential functions on the right-hand side in the second equations were corrected.

On p. 372, right column, an error is involved in equation (22a). It must be corrected to

$$\begin{aligned} I_{og'}(\mathbf{r}) &= \frac{1}{4}\frac{\gamma_o}{\gamma_g} \exp\left[-\frac{1}{2}\mu_o\left(\frac{1}{\gamma_o} + \frac{1}{\gamma_g}\right)(t_1 + t_2)\right] \frac{U_r^2}{u_{or}^2 + U_r^2} \\ &\quad \times \left[\left(1 + \frac{u_r^2}{u_r^2 + U_r^2}\right)\cosh(2K\alpha_{21,i}t_1) + \frac{2u_r}{(u_r^2 + U_r^2)^{1/2}} \right. \\ &\quad \left. \times \sinh(2K\alpha_{21,i}t_1) + \frac{U_r^2}{u_r^2 + U_r^2}\cos(2K\alpha_{21,r}t_1)\right] \\ &\quad \times \big[\cosh(2K\beta_{o,i}t_2) - \cos(2K\beta_{o,r}t_2)\big]. \end{aligned} \tag{22a}$$

In this correction, the last term in the second bracket on the right-hand side was corrected. On p. 373, left column, equation (24b) is incorrect. It must be corrected to



$$K\alpha_{21,i} = \frac{1}{2}\frac{(u_r u_i + U_r U_i)}{(u_r^2 + U_r^2)^{1/2}}\frac{1}{\gamma_g}. \qquad (24b)$$

On p. 376, left column, the description of '$t_{\rm gap}$ = 0.024 mm' is incorrect. It must be corrected to '$t_{\rm gap}$ = 0.24 mm'. The mentioned errors in equations (14*b*), (14*c*) and (24*b*) do not influence the calculation of equations (20) to (23*b*), since the correct expressions as above were used in deriving them. The mentioned error in equation (22*a)* does not influence the computations of the presented images and graphs in the paper, since the computations were all made correctly using the correct expression as mentioned above; the errors are only in the text.

As a supplement to the previous presentation of the equation for the diffracted – or G – wave image intensity $I_g(\mathbf{r})$ in equation (20), the equation for the corresponding transmitted – or O – wave image intensity $I_o(\mathbf{r})$ is added as in the following:

$$\begin{aligned} I_o(\mathbf{r}) &= \left|\sum_{i,j}\left[E_{oo'}^{i,j}(\mathbf{r}) + E_{go'}^{i,j}(\mathbf{r})\right]\right|^2 \\ &= I_{oo'}(\mathbf{r}) + I_{go'}(\mathbf{r}) + A_o(\mathbf{r})\cos\Psi_o(\mathbf{r}) + B_o(\mathbf{r})\sin\Psi_o(\mathbf{r}) \end{aligned} \qquad (49)$$

with

$$\begin{aligned} \Psi_o(\mathbf{r}) &= 2\pi[\Delta\mathbf{g}\cdot(\mathbf{r}-\mathbf{r}_o)] + K\alpha_{go}t_2 - u_n t_{\rm gap}/\gamma_g \\ &\quad - 2\pi(\Delta\mathbf{g}\cdot\hat{\mathbf{K}}_o)\cdot(T_{b'}/\gamma_o) \end{aligned} \qquad (50)$$

$$\begin{aligned} I_{oo'}(\mathbf{r}) &= \frac{1}{4}\exp\left[-\frac{1}{2}\mu_o\left(\frac{1}{\gamma_o}+\frac{1}{\gamma_g}\right)(t_1+t_2)\right] \\ &\quad\times\left[\left(1+\frac{u_r^2}{u_r^2+U_r^2}\right)\cosh(2K\alpha_{21,i}t_1) + \frac{2u_r}{(u_r^2+U_r^2)^{1/2}}\right. \\ &\quad\left.\times\sinh(2K\alpha_{21,i}t_1) + \frac{U_r^2}{u_r^2+U_r^2}\cos(2K\alpha_{21,r}t_1)\right] \\ &\quad\times\left[\left(1+\frac{u_{or}^2}{u_{or}^2+U_r^2}\right)\cosh(2K\beta_{o,i}t_2) + \frac{2u_{or}}{(u_{or}^2+U_r^2)^{1/2}}\right. \\ &\quad\left.\times\sinh(2K\beta_{o,i}t_2) + \frac{U_r^2}{u_{or}^2+U_r^2}\cos(2K\beta_{o,r}t_2)\right] \end{aligned} \qquad (51a)$$

$$\begin{aligned} I_{go'}(\mathbf{r}) &= \frac{1}{4}\exp\left[-\frac{1}{2}\mu_o\left(\frac{1}{\gamma_o}+\frac{1}{\gamma_g}\right)(t_1+t_2)\right] \\ &\quad\times\frac{U_r^2}{(u_r^2+U_r^2)}\frac{U_r^2}{(u_{gr}^2+U_r^2)}\left[\cosh(2K\alpha_{21,i}t_1)\right. \\ &\quad\left.-\cos(2K\alpha_{21,r}t_1)\right]\left[\cosh(2K\beta_{g,i}t_2)-\cos(2K\beta_{g,r}t_2)\right] \end{aligned} \qquad (51b)$$

$$\begin{aligned} A_o(\mathbf{r}) &= \frac{1}{2}\exp\left[-\frac{1}{2}\mu_o\left(\frac{1}{\gamma_o}+\frac{1}{\gamma_g}\right)(t_1+t_2)\right] \\ &\quad\times\frac{U_r}{(u_r^2+U_r^2)^{1/2}}\frac{U_r}{(u_{gr}^2+U_r^2)^{1/2}}\Big\{\{\sinh(2K\alpha_{21,i}t_1) \\ &\quad\times[\cos(K\beta_{-,r}t_2)\sinh(K\beta_{+,i}t_2)+\cos(K\beta_{+,r}t_2) \\ &\quad\times\sinh(K\beta_{-,i}t_2)] - \sin(2K\alpha_{21,r}t_1)[\sin(K\beta_{-,r}t_2) \\ &\quad\times\cosh(K\beta_{+,i}t_2)+\sin(K\beta_{+,r}t_2)\cosh(K\beta_{-,i}t_2)]\} \\ &\quad+\frac{u_{or}}{(u_{or}^2+U_r^2)^{1/2}}\{\sinh(2K\alpha_{21,i}t_1)[\cos(K\beta_{-,r}t_2) \\ &\quad\times\cosh(K\beta_{+,i}t_2)-\cos(K\beta_{+,r}t_2)\cosh(K\beta_{-,i}t_2)] \\ &\quad-\sin(2K\alpha_{21,r}t_1)\cdot[\sin(K\beta_{-,r}t_2)\sinh(K\beta_{+,i}t_2) \\ &\quad-\sin(K\beta_{+,r}t_2)\sinh(K\beta_{-,i}t_2)]\} \\ &\quad+\frac{u_r}{(u_r^2+U_r^2)^{1/2}}[\cosh(2K\alpha_{21,i}t_1)-\cos(2K\alpha_{21,r}t_1)] \\ &\quad\times[\cos(K\beta_{-,r}t_2)\sinh(K\beta_{+,i}t_2)+\cos(K\beta_{+,r}t_2) \\ &\quad\times\sinh(K\beta_{-,i}t_2)]+\frac{u_r}{(u_r^2+U_r^2)^{1/2}}\frac{u_{or}}{(u_{or}^2+U_r^2)^{1/2}} \\ &\quad\times[\cosh(2K\alpha_{21,i}t_1)-\cos(2K\alpha_{21,r}t_1)] \\ &\quad\times[\cos(K\beta_{-,r}t_2)\cosh(K\beta_{+,i}t_2)-\cos(K\beta_{+,r}t_2) \\ &\quad\times\cosh(K\beta_{-,i}t_2)]\Big\} \end{aligned} \qquad (52a)$$

$$\begin{aligned} B_o(\mathbf{r}) &= \frac{1}{2}\exp\left[-\frac{1}{2}\mu_o\left(\frac{1}{\gamma_o}+\frac{1}{\gamma_g}\right)(t_1+t_2)\right] \\ &\quad\times\frac{U_r}{(u_r^2+U_r^2)^{1/2}}\frac{U_r}{(u_{gr}^2+U_r^2)^{1/2}}\Big\{\{-\sinh(2K\alpha_{21,i}t_1) \\ &\quad\times[\sin(K\beta_{-,r}t_2)\cosh(K\beta_{+,i}t_2)+\sin(K\beta_{+,r}t_2) \\ &\quad\times\cosh(K\beta_{-,i}t_2)] - \sin(2K\alpha_{21,r}t_1)[\cos(K\beta_{-,r}t_2) \\ &\quad\times\sinh(K\beta_{+,i}t_2)+\cos(K\beta_{+,r}t_2)\sinh(K\beta_{-,i}t_2)]\} \\ &\quad+\frac{u_{or}}{(u_{or}^2+U_r^2)^{1/2}}\{-\sinh(2K\alpha_{21,i}t_1)[\sin(K\beta_{-,r}t_2) \\ &\quad\times\sinh(K\beta_{+,i}t_2)-\sin(K\beta_{+,r}t_2)\sinh(K\beta_{-,i}t_2)] \\ &\quad-\sin(2K\alpha_{21,r}t_1)\cdot[\cos(K\beta_{-,r}t_2)\cosh(K\beta_{+,i}t_2) \\ &\quad-\cos(K\beta_{+,r}t_2)\cosh(K\beta_{-,i}t_2)]\} \\ &\quad-\frac{u_r}{(u_r^2+U_r^2)^{1/2}}[\cosh(2K\alpha_{21,i}t_1)-\cos(2K\alpha_{21,r}t_1)] \\ &\quad\times[\sin(K\beta_{-,r}t_2)\cosh(K\beta_{+,i}t_2)+\sin(K\beta_{+,r}t_2) \\ &\quad\times\cosh(K\beta_{-,i}t_2)]-\frac{u_r}{(u_r^2+U_r^2)^{1/2}}\frac{u_{or}}{(u_{or}^2+U_r^2)^{1/2}} \\ &\quad\times[\cosh(2K\alpha_{21,i}t_1)-\cos(2K\alpha_{21,r}t_1)] \\ &\quad\times[\sin(K\beta_{-,r}t_2)\sinh(K\beta_{+,i}t_2)-\sin(K\beta_{+,r}t_2) \\ &\quad\times\sinh(K\beta_{-,i}t_2)]\Big\}. \end{aligned} \qquad (52b)$$

The numbering of the equations here is continued from the last equation (48) in the original paper (Yoshimura, 2015). $E_{oo'}^{i,j}(\mathbf{r})$ and $E_{go'}^{i,j}(\mathbf{r})$ in equation (49) are as given in equations (14*a*), (14*c*), respectively.

Through similar calculations to those written in the right-hand side column on p. 373, the term of interference phase $\Psi_o(\mathbf{r})$ in equation (50) can be reduced to

$$\Psi_o(\mathbf{r}) = \Psi_o(\mathbf{r}_{b'}) = \{2\pi\Delta\mathbf{g}_{\parallel} \cdot [(\mathbf{r}_{b'} - \mathbf{r}_o)_{\parallel} - \mathbf{l}_{\parallel}] - u_n t_{\rm gap}/\gamma_g\} \quad (53)$$

which is the same as $\Psi_g(\mathbf{r})$ in equation (34) for the G-wave image intensity (here, the symbol $\parallel$ denotes the component parallel to the specimen surfaces). In the present case that $(\mathbf{r} - \mathbf{r}_{b'}) \parallel \hat{\mathbf{K}}_o$, part of the first term and the fourth term in equation (50) cancel each other as follows:

$$\begin{aligned} &2\pi[\Delta\mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{b'})] - 2\pi(\Delta\mathbf{g} \cdot \hat{\mathbf{K}}_o)(T_{b'}/\gamma_o) \\ &= 2\pi[\Delta\mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{b'})] - 2\pi(\Delta\mathbf{g} \cdot \hat{\mathbf{K}}_o) \cdot [(\mathbf{r} - \mathbf{r}_{b'}) \cdot \mathbf{n}]/(\hat{\mathbf{K}}_o \cdot \mathbf{n}) \\ &= 0. \end{aligned}$$

The moiré images of the O-wave in Figs. 14(a) and 14(b) and the curves concerned in Figs. 15(a) and 15(b) were computed using these equations (49), (51a)–(52b) and (53).

References

Yoshimura, J. (2015). *Acta Cryst.* A**71**, 368–381.