Ultramicroscopy 32 (1990) 297–298
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ADDENDUM

J.E. Bonevich and L.D. Marks, Contrast transfer theory for non-linear imaging. Ultramicroscopy 26 (1988) 313.

Our original manuscript contained an analytical solution of the transmission cross-coefficient that included the second-order terms of the beam convergence. However, the cross-terms between the focal spread and convergence can also be included in the solution.

Starting with the complete equation for the transmission cross-coefficient in reduced units,

$$T(\boldsymbol{u}, \boldsymbol{q}, \Delta z) = \int\int \exp\big\{(i\pi/2)\big\{2(\Delta z + f)\big[q^2 + 2\boldsymbol{w}\cdot(\boldsymbol{u}-\boldsymbol{q}) - u^2\big]$$
$$+\big[q^4 - 2w^2(u^2 - q^2) - u^4 + 4\boldsymbol{w}\cdot(u^2\boldsymbol{u} - q^2\boldsymbol{q})$$
$$-4(|\boldsymbol{u}\cdot\boldsymbol{w}|^2 - |\boldsymbol{q}\cdot\boldsymbol{w}|^2) + 4w^2\boldsymbol{w}\cdot(\boldsymbol{u}-\boldsymbol{q})\big]\big\}\big\}$$
$$\times\sqrt{\beta/\pi}\exp(-\beta f^2)\,\mathrm{d}f\;(\alpha/\pi)\exp(-\alpha w^2)\,\mathrm{d}\boldsymbol{w}.$$

If we first consider the integration over f, the envelope term for the focal spread is:

$$\exp\big\{-(\pi^2/4\beta)\big[q^4 - 2u^2q^2 + u^4 - 4\boldsymbol{w}\cdot(\boldsymbol{u}-\boldsymbol{q})(u^2-q^2) + 4|\boldsymbol{w}\cdot(\boldsymbol{u}-\boldsymbol{q})|^2\big]\big\}.$$

The constant terms,

$$(\alpha/\pi)\exp\big[-\pi^2(q^2-u^2)^2/4\beta\big],$$

are removed from the integral. Now including the cross-terms between the focal spread and convergence, the $\Delta\alpha$ interaction [1] leaves

$$\int\exp\big(i\boldsymbol{w}\cdot\big[\nabla\chi(\boldsymbol{u}) - \nabla\chi(\boldsymbol{q}) - i(\pi^2/\beta)(u^2-q^2)(\boldsymbol{u}-\boldsymbol{q})\big]$$
$$-w^2\big\{\alpha + (\pi^2/\beta)|\boldsymbol{u}-\boldsymbol{q}|^2 + i\pi\big[u^2 - q^2 + (2/w^2)(|\boldsymbol{u}\cdot\boldsymbol{w}|^2 - |\boldsymbol{q}\cdot\boldsymbol{w}|^2) - 2\boldsymbol{w}\cdot(\boldsymbol{u}-\boldsymbol{q})\big]\big\}\big)\,\mathrm{d}\boldsymbol{w}.$$

The integral is then split into the x and y components as before.

$$\int\exp\big(i\boldsymbol{x}\cdot\big[\nabla\chi(\boldsymbol{u}) - \nabla\chi(\boldsymbol{q}) - i(\pi^2/\beta)(u^2-q^2)(\boldsymbol{u}-\boldsymbol{q})\big]$$
$$-x^2\big\{\alpha + (\pi^2/\beta)|\boldsymbol{u}-\boldsymbol{q}|^2 + i\pi\big[u^2(1+2\cos^2\Theta_2) - q^2(1+2\cos^2\Theta_3) - 2\boldsymbol{x}\cdot(\boldsymbol{u}-\boldsymbol{q})\big]\big\}\big)\,\mathrm{d}x$$
$$\times\int\exp\big(i\boldsymbol{y}\cdot\big[\nabla\chi(\boldsymbol{u}) - \nabla\chi(\boldsymbol{q})\big] - y^2\big\{\alpha + i\pi\big[u^2(1+2\sin^2\Theta_2) - q^2(1+2\sin^2\Theta_3)\big]\big\}\big)\,\mathrm{d}y.$$

Note that the cross-terms between the spatial and temporal coherence only are present in the integral over x (parallel to $\boldsymbol{v} = \boldsymbol{u} - \boldsymbol{q}$). These additional terms can be included in the analytical solution for $T(\boldsymbol{u}, \boldsymbol{q}, \Delta z)$

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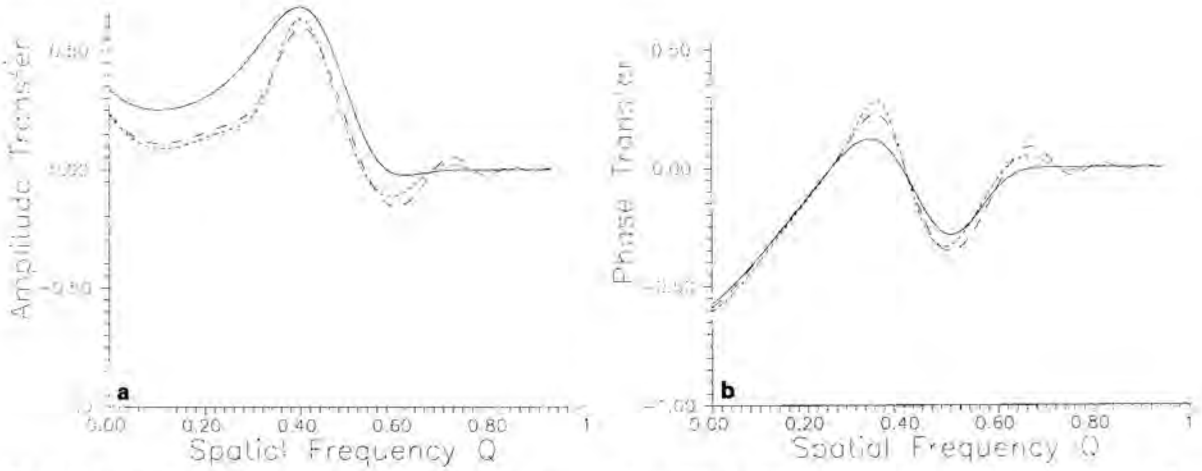

Fig. 1. Non-linear interference with g_{100} along parallel orientations for original solution (short dashes), the $\Delta\alpha$ cross-terms included (long dashes), and the full solution (solid). The rms focal spread was 70 Å, rms convergence of 3 mrad, electron energy of 300 keV, C_s of 0.9 mm, at −500 Å underfocus.

provided that we neglect the cubic term of w:

$$\begin{aligned} T(\boldsymbol{u}, \boldsymbol{q}, \Delta z) &= \exp[-\mathrm{i}\chi(\boldsymbol{u}) + \mathrm{i}\chi(\boldsymbol{q})] \exp\left\{-\left[\pi^2(q^2-u^2)^2/4\beta\right]\right\} \\ &\times \exp\Big(-\left[\nabla\chi(\boldsymbol{u}) \cos\Theta_2 - \nabla\chi(\boldsymbol{q}) \cos\Theta_3 - \mathrm{i}(\pi^2/\beta)(u^2-q^2)\,|\boldsymbol{u}-\boldsymbol{q}|\right]^2 \\ &/4\left\{\alpha + (\pi^2/\beta)\,|\boldsymbol{u}-\boldsymbol{q}|^2 + \mathrm{i}\pi\left[u^2(1+2\cos^2\Theta_2) - q^2(1+2\cos^2\Theta_3)\right]\right\}\Big) \\ &\times \exp\Big(-\left[\nabla\chi(\boldsymbol{u}) \sin\Theta_2 + \nabla\chi(\boldsymbol{q}) \sin\Theta_3\right]^2 \\ &/4\left\{\alpha + \mathrm{i}\pi\left[u^2(1+2\sin^2\Theta_2) - q^2(1+2\sin^2\Theta_3)\right]\right\}\Big) \\ &\times \alpha/\Big(\left\{\alpha + (\pi^2/\beta)\,|\boldsymbol{u}-\boldsymbol{q}|^2 + \mathrm{i}\pi\left[u^2(1+2\cos^2\Theta_2) - q^2(1+2\cos^2\Theta_3)\right]\right\} \\ &\times \left\{\alpha + \mathrm{i}\pi\left[u^2(1+2\sin^2\Theta_2) - q^2(1+2\sin^2\Theta_3)\right]\right\}\Big)^{1/2}. \end{aligned}$$

As before, the full solution can be found by numerical integration.

Fig. 1 shows the results for the original test case. While the full integration represents the true solution, there are only subtle differences between the solution containing the $\Delta\alpha$ cross-terms and the original analytical solution. The cross-terms become significant in the extreme case of high focal spread and convergence. In any event, the improved solution represents a substantial improvement over first-order non-linear theory.

The authors would like to thank Dr. M.A. O'Keefe for correspondence leading to this addendum.

Reference

[1] M.A. O'Keefe, in: Proc. 37th Annu. EMSA Meeting, 1979, Ed. G.W. Bailey, p. 556.