Journal of
Applied
Crystallography
ISSN 1600-5767

addenda and errata

Elastic strain and stress determination by Rietveld refinement: generalized treatment for textured polycrystals for all Laue classes. Second corrigendum

N. C. Popa[a] and D. Balzar[b]*

[a]National Institute for Materials Physics, PO Box MG 7, Bucharest, Romania, and [b]Department of Physics and Astronomy, University of Denver, 2112 East Wesley Avenue, Denver, CO 80208, USA. Correspondence e-mail: balzar@du.edu

This corrigendum (C2) replaces the first corrigendum (C1; Popa & Balzar, 2012), which was published to correct errors in the article by Popa & Balzar (2001). The basic equation considered in C1 is the integral of spherical harmonics over the crystallites contributing to the Bragg reflection. In C1, this integral is represented by equation (1), which is the expression (14.160) originally calculated by Bunge (1982). In C1, we added the factor $(-1)^n$ to that expression. This factor resulted from a coding error that, unfortunately, we discovered only recently in the computer routine used to calculate such integrals. With the correct coding, the factor $(-1)^n$ disappears, and the Bunge (1982) equation (14.120) is correct.

The necessary corrections in the paper by Popa & Balzar (2001) are the following:

(1) Table 1: multiply the right side of each equation by 2.

(2) Table 15: delete the factor 2 in the right side of the equations for R_0 and R_1.

(3) Several errors in Table 16. The correct table is shown as Table 1 of the present article.

(4) The first unnumbered equation after equation (24) becomes $g'_{jk} = \sum_{l=1}^{6} C_{jl}\,\rho_l\,g_{lk}$.

References

Bunge, H. I. (1982). *Texture Analysis in Materials Science*. London: Butterworth.
Popa, N. C. & Balzar, D. (2001). *J. Appl. Cryst.* **34**, 187–195.
Popa, N. C. & Balzar, D. (2012). *J. Appl. Cryst.* **45**, 838–839.

Table 1
The corrected version of Table 16.

$k = 0:$	$\bar{w}_{ij0} = 1/3$ for $i, j = 1, 3$
$k = 1:$	$\bar{w}_{ij1} = 1/30$ for $i, j = 1, 2$; $\bar{w}_{ij1} = 2/15$ for $(3, 3)$; $\bar{w}_{ij1} = -1/15$ for $(1, 3), (2, 3), (3, 1), (3, 2)$
$k = 2:$	$\bar{w}_{ij2} = -1/30(3/2)^{1/2}$ for $(5, 1), (5, 2)$; $\bar{w}_{ij2} = 1/15(3/2)^{1/2}$ for $(5, 3)$
$k = 3:$	$\bar{w}_{ij3} = -1/30(3/2)^{1/2}$ for $(4, 1), (4, 2)$; $\bar{w}_{ij2} = 1/15(3/2)^{1/2}$ for $(4, 3)$
$k = 4:$	$\bar{w}_{ij4} = -1/30(3/2)^{1/2}$ for $(1, 1), (1, 2)$; $\bar{w}_{ij4} = 1/15(3/2)^{1/2}$ for $(1, 3)$; $\bar{w}_{ij4} = 1/30(3/2)^{1/2}$ for $(2, 1), (2, 2)$; $\bar{w}_{ij4} = -1/15(3/2)^{1/2}$ for $(2, 3)$
$k = 5:$	$\bar{w}_{ij5} = -1/30(3/2)^{1/2}$ for $(6, 1), (6, 2)$; $\bar{w}_{ij5} = 1/15(3/2)^{1/2}$ for $(6, 3)$
$k = 6:$	$\bar{w}_{ij6} = -1/15(3/2)^{1/2}$ for $(1, 5), (2, 5)$; $\bar{w}_{ij6} = 2/15(3/2)^{1/2}$ for $(3, 5)$
$k = 7:$	$\bar{w}_{ij7} = 1/10$ for $(5, 5)$
$k = 8:$	$\bar{w}_{ij8} = 1/10$ for $(4, 5)$
$k = 9:$	$\bar{w}_{ij9} = 1/10$ for $(1, 5)$; $\bar{w}_{ij9} = -1/10$ for $(2, 5)$
$k = 10:$	$\bar{w}_{ij,10} = 1/10$ for $(6, 5)$
$k = 11:$	$\bar{w}_{ij,11} = -1/15(3/2)^{1/2}$ for $(1, 4), (2, 4)$; $\bar{w}_{ij,11} = 2/15(3/2)^{1/2}$ for $(2, 4)$
$k = 12:$	$\bar{w}_{ij,12} = 1/10$ for $(5, 4)$
$k = 13:$	$\bar{w}_{ij,13} = 1/10$ for $(4, 4)$
$k = 14:$	$\bar{w}_{ij,14} = 1/10$ for $(1, 4)$; $\bar{w}_{ij,14} = -1/10$ for $(2, 4)$
$k = 15:$	$\bar{w}_{ij,15} = 1/10$ for $(6, 4)$
$k = 16:$	$\bar{w}_{ij,16} = -1/30(3/2)^{1/2}$ for $(1, 1), (2, 1)$; $\bar{w}_{ij,16} = 1/30(3/2)^{1/2}$ for $(1, 2), (2, 2)$; $\bar{w}_{ij,16} = 1/15(3/2)^{1/2}$ for $(3, 1)$; $\bar{w}_{ij,16} = -1/15(3/2)^{1/2}$ for $(3, 2)$
$k = 17:$	$\bar{w}_{ij,17} = 1/20$ for $(5, 1)$; $\bar{w}_{ij,17} = -1/20$ for $(5, 2)$
$k = 18:$	$\bar{w}_{ij,18} = 1/20$ for $(4, 1)$; $\bar{w}_{ij,18} = -1/20$ for $(4, 2)$
$k = 19:$	$\bar{w}_{ij,19} = 1/20$ for $(1, 1), (2, 2)$; $\bar{w}_{ij,19} = -1/20$ for $(1, 2), (2, 1)$
$k = 20:$	$\bar{w}_{ij,20} = 1/20$ for $(6, 1)$; $\bar{w}_{ij,20} = -1/20$ for $(6, 2)$
$k = 21:$	$\bar{w}_{ij,21} = -1/15(3/2)^{1/2}$ for $(1, 6), (2, 6)$; $\bar{w}_{ij,21} = 2/15(3/2)^{1/2}$ for $(3, 6)$
$k = 22:$	$\bar{w}_{ij,22} = 1/10$ for $(5, 6)$
$k = 23:$	$\bar{w}_{ij,23} = 1/10$ for $(4, 6)$
$k = 24:$	$\bar{w}_{ij,24} = 1/10$ for $(1, 6)$; $\bar{w}_{ij,24} = -1/10$ for $(2, 6)$
$k = 25:$	$\bar{w}_{ij,25} = 1/10$ for $(6, 6)$

 doi:10.1107/S1600576714022109