Short Communication

Symmetry requirements of W_{lmn} with odd l for cubic crystal symmetry

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While X-ray pole-figure measurements only permit direct determination of C_l^{mn} (Bunge, 1965, 1969) or W_{lmn} (Roe, 1965, 1966), with even l , the need for such coefficients with odd l has recently been pointed out by Matthies (1979). Methods for determining such coefficients have been suggested by Bunge and Esling (1979), Matthies and Pospiech (1980), and Lücke *et al.* (1980). Implementation of such methods for cubic crystal symmetry requires a knowledge of either the symmetric generalized spherical harmonics (Bunge) or the relation between linearly dependent and linearly independent coefficients imposed by crystal symmetry operations (Roe). In this communication the process adopted by Roe (1966) for even l has been extended to odd l . This results in $W_{lmo} = 0$ for odd l . The results of computer calculations for Roe's Eq. (7) with odd l are summarized in Table I. Double precision arithmetic was used throughout the calculation, and the figures given in Table I are correct within half a unit in the last significant digit. The augmented Jacobi polynomials, $Z_{lmn}(\xi)$, may be calculated using the program published by Morris (1975), or a modification of that published by Pospiech and Jura (1975). The sign of $Z_{lmn}(\xi)$ for even, odd l, m, n has been discussed by Morris and Koskenmaki (1977).

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TABLE I
Relations between W_{lmn} with odd l for cubic crystal symmetry

l	Linearly indep. coeff.	Linearly depend. coeff.
9	W_{9m4}	$W_{9m8} = -0.64168895 W_{9m4}$
13	W_{13m4}	$W_{13m8} = 0.29019050 W_{13m4}$ $W_{13m12} = -0.72981613 W_{13m4}$
15	W_{15m4}	$W_{15m8} = -2.7026557 W_{15m4}$ $W_{15m12} = 1.6810970 W_{15m4}$
17	W_{17m4}	$W_{17m8} = 0.47548602 W_{17m4}$ $W_{17m12} = 0.05194854 W_{17m4}$ $W_{17m16} = -0.78325810 W_{17m4}$
19	W_{19m4}	$W_{19m8} = -1.6733200 W_{19m4}$ $W_{19m12} = -0.82826415 W_{19m4}$ $W_{19m16} = 1.4561697 W_{19m4}$
21	W_{21m4} W_{21m8}	$W_{21m12} = 1.1297868 W_{21m4} - 1.5862311 W_{21m8}$ $W_{21m16} = -0.61409748 W_{21m4} + 0.98152062 W_{21m8}$ $W_{21m20} = -0.67564597 W_{21m4} - 0.26207622 W_{21m8}$
23	W_{23m4}	$W_{23m8} = -1.1699216 W_{23m4}$ $W_{23m12} = -1.0389292 W_{23m4}$ $W_{23m16} = -0.17708075 W_{23m4}$ $W_{23m20} = 1.3143848 W_{23m4}$

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