

Table 3. Results of simulations investigating distribution of  $d_w$  as a function of  $\sigma(\mu)$

See text for explanation of symbols. Table gives percentage of simulated  $|d_w|$  values that exceeded  $z_{0.05}$  ( $=1.96$ ).

$\sigma(\mu)$	Sample size	$\sigma_{\min}-\sigma_{\max}$		
		0.001-0.005	0.001-0.010	0.001-0.030
0.0	$k=5$	4.4	5.4	4.6
	$k=10$	5.2	5.3	5.1
	$k=20$	4.9	5.0	4.9
$\frac{\sigma_{\min} + \sigma_{\max}}{8}$	$k=5$	6.9	10.4	18.3
	$k=10$	7.1	11.4	24.9
	$k=20$	7.3	12.8	30.3
$\frac{\sigma_{\min} + \sigma_{\max}}{4}$	$k=5$	13.4	20.9	31.6
	$k=10$	14.1	24.3	42.4
	$k=20$	15.6	28.9	51.6
$\frac{\sigma_{\min} + \sigma_{\max}}{2}$	$k=5$	30.1	41.5	52.8
	$k=10$	33.0	50.0	61.9
	$k=20$	35.6	52.5	71.8

extremely sensitive to the presence of environmental effects. For example, with the simulation parameters given above, some 30% of the  $d_w$  values were formally significant at the 95% confidence level (i.e. the true confidence level of the test was about 70%). We conclude that the use of weighted means in hypothesis tests is extremely dangerous when  $\sigma(\mu)$  is not negligibly small.

#### IV. Conclusions

In our previous study (Taylor & Kennard, 1983) we concluded that the unweighted mean is probably satisfactory for most samples of crystallographic data. The present work reinforces this conclusion since it shows that unweighted means may be used in hypothesis tests with little difficulty. Some approximations are necessary when environmental effects are small, but they are unlikely to cause problems in practice. In contrast, the use of  $d_w$  in hypothesis tests cannot be recommended. This is mainly because the value of  $\sigma(\bar{x}_w)$  obtained from (5) may be a gross underestimate of the true standard error of the weighted mean if environmental effects are not negligible.

Olga Kennard is a member of the external staff of the Medical Research Council.

#### References

- COCHRAN, W. G. (1954). *Biometrics*, **10**, 101-129.  
 COCHRAN, W. G. & CARROLL, S. P. (1953). *Biometrics*, **9**, 447-459.  
 CRUICKSHANK, D. W. J. & ROBERTSON, A. P. (1953). *Acta Cryst.* **6**, 698-705.  
 HAMILTON, W. C. & ABRAHAMS, S. C. (1970). *Acta Cryst.* **A26**, 18-24.  
 NAG Fortran Library Manual (1983). Mark 10, Vol. 5.  
 STUDENT (1908). *Biometrika*, **6**, 1-25.  
 TAYLOR, R. & KENNARD, O. (1983). *Acta Cryst.* **B39**, 517-525.  
 TAYLOR, R. & KENNARD, O. (1985). In preparation.

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**Tensorial classification of non-magnetic ferroic crystals: tensors of rank  $N \leq 4$ .** By D. B. LITVIN, Department of Physics, The Pennsylvania State University, The Berks Campus, PO Box 2150, Reading, PA 19608, USA

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#### Abstract

The tensorial classification of all non-magnetic ferroic crystals is given for all possible macroscopic tensorial properties of rank  $N \leq 4$ .

A ferroic crystal can be classified according to the point-group symmetry of the non-ferroic or prototypic phase and the point-group symmetries of the ferroic crystal's domains. Each class of ferroic crystals is denoted by a symbol **GFH**, where **F** is a symbol denoting 'ferroic', **G** the point group of the non-ferroic phase, and **H** the point group of one of

the ferroic crystal's domains (Aizu, 1970, 1976*a,b*). The domains of a ferroic crystal can possibly be distinguished by the values of the components of a macroscopic tensorial property associated with each of the domains. Whether or not one can distinguish some or all of the domains has led to the additional tensorial classification of ferroic crystals (Aizu, 1969, 1970). Aizu has tabulated the magnetic classes of ferroic crystals and the tensorial classification of ferroelectric, ferromagnetic and ferroelastic crystals (Aizu, 1970; see also Cracknell, 1972). A method has been presented (Litvin, 1984) to determine the tensorial classification of non-magnetic ferroic crystals for an arbitrary tensorial property.

Consider a ferroic crystal belonging to the ferroic class  $\mathbf{GFH}$  and let  $|\mathbf{G}|$  and  $|\mathbf{H}|$  denote the order of the groups  $\mathbf{G}$  and  $\mathbf{H}$ , respectively. The number  $n$  of domains of the ferroic crystal is given by  $n = |\mathbf{G}|/|\mathbf{H}|$ . The point group  $\mathbf{G}$  can be written in a coset decomposition with respect to the proper subgroup  $\mathbf{H}$ :

$$\mathbf{G} = \mathbf{H} + G_2\mathbf{H} + \dots + G_n\mathbf{H}. \quad (1)$$

Consider a ferroic crystal of the ferroic class  $\mathbf{GFH}$  and a macroscopic tensorial property represented by a  $q$ -component tensor  $\mathbf{T}$ . We denote the components of  $\mathbf{T}$  by  $T_j$ ,  $j = 1, 2, \dots, q$ . The  $n$  sets of values of the components of  $\mathbf{T}$  characterizing the  $n$  domains of the ferroic crystal are denoted by (Nye, 1964)

$$\{T_j\}, \{G_2T_j\}, \dots, \{G_nT_j\}. \quad (2)$$

The set  $\{G_iT_j\}$  of the components of the tensor  $\mathbf{T}$  corresponding to the  $i$ th domain is related to the set  $\{T_j\}$  by the  $i$ th coset representative  $G_i$  of (1) (Litvin, 1984).

Ferroic crystals are given a tensorial classification, with respect to a given tensor  $\mathbf{T}$ , according to one's ability to distinguish among the domains by considering only the sets of values, (2), of the components of the macroscopic tensorial property: ferroic crystals of a ferroic class  $\mathbf{GFH}$  are said to belong to a

(1) 'full' ferroic class with respect to the tensor  $\mathbf{T}$  if the sets of values of the components of  $\mathbf{T}$  characterizing the  $n$  domains, (2), are all distinct;

(2) 'partial' ferroic class with respect to the tensor  $\mathbf{T}$  if only  $m$ ,  $1 < m < n$ , of the sets in (2) are distinct;

(3) 'null' ferroic class with respect to the tensor  $\mathbf{T}$  if all sets in (2) are identical.

The terminology full, partial and null was introduced by Aizu (1969, 1970). We shall subdivide the third classification into two: ferroic crystals of a ferroic class  $\mathbf{GFH}$  will be said to belong to a

(3a) 'null' ferroic class with respect to the tensor  $\mathbf{T}$  if all sets in (2) are identical and non-zero.

(3b) 'zero' ferroic class with respect to the tensor  $\mathbf{T}$  if all sets in (2) are identically zero.

We have applied the method of Litvin (1984) to determine the tensorial classification of all ferroic classes of non-magnetic ferroic crystals for all macroscopic tensorial properties represented by tensors of rank zero through four.

Tensorial properties are characterized by the transformational properties of their components with respect to the full rotation group  $\mathbf{R}$ . The components  $T_j$ ,  $j = 1, 2, \dots, q$ , of the tensor  $\mathbf{T}$  are basic functions of a representation  $D^T$  of  $\mathbf{R}$ :

$$RT_j = \sum_k D^T(R)_{kj} T_k. \quad (3)$$

The representation  $D^T$  is in general a reducible representation of  $\mathbf{R}$ ,

$$D^T(R) = \sum_i a_i D^i(R), \quad (4)$$

where  $a_i$  is the number of times the irreducible representation  $D^i$  of  $\mathbf{R}$  appears in the reduced form of  $D^T$ . The tensorial classification of a ferroic crystal with respect to a tensor  $\mathbf{T}$  depends (Litvin, 1984) only on the set of irreducible representations with non-zero coefficients appearing in (4). For tensor of rank zero through four there are 62 possible sets of irreducible representations of  $\mathbf{R}$  appearing in (4). The decomposition, (4), for tensors of rank two, three and four of various intrinsic symmetries has been given by Tenenbaum (1966). We have tabulated the tensorial classification of all 247 non-magnetic classes of ferroic crystals with respect to tensors corresponding to each of the 62 possible sets of irreducible representations.\*

\* The complete tables have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39619 (88 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

#### References

- AIZU, K. (1969). *J. Phys. Soc. Jpn*, **27**, 387-396.  
 AIZU, K. (1970). *Phys. Rev. B*, **2**, 754-772.  
 AIZU, K. (1976a). *J. Phys. Soc. Jpn*, **40**, 371-376.  
 AIZU, K. (1976b). *J. Phys. Soc. Jpn*, **41**, 1-8.  
 CRACKNELL, A. P. (1972). *Acta Cryst.* **A28**, 597-601.  
 LITVIN, D. B. (1984). *Acta Cryst.* **A40**, 255-261.  
 NYE, J. F. (1964). *Physical Properties of Crystals*. Oxford: Clarendon Press.  
 TENENBAUM, J. (1966). *Proc. Indian Acad. Sci.* **64**, 74-83.