

3. SYMMETRY ASPECTS OF PHASE TRANSITIONS, TWINNING AND DOMAIN STRUCTURES

integrity basis of polynomial invariants and of the linear bases of polynomial covariants.

(3) *Twinning group*: This option works for the first group of the set of conjugate subgroups only. It displays a table that contains consecutive normalizers of the set of conjugate subgroups, left, right and double coset resolutions of the parent group G with respect to the subgroup F_1 , and the twinning groups assigned to double cosets. This is the basic information concerning pairs of domain states.

Lattices of equitranslational subgroups of the space groups. The importance of these lattices was realized by Ascher (1968), who prepared the first tables. However, his tables do not contain full information about subgroups; neither the parent group nor the subgroups are completely specified. The current version gives the full information about subgroups including their settings and origins. The pull-down menu *Groups* contains two options: *Point* and *Space*. The choice of the second option brings to the screen another panel, in the right-hand part of which are listed space groups of the geometric class G through Hermann–Mauguin symbols corresponding to all settings and cell choices where applicable. The number of the space-group type, the Schoenflies symbol, the setting and the cell choice are shown in the left-hand part of the panel when you click on one of these Hermann–Mauguin symbols. At the same time, the symbols of the point groups in the lattice change to Schoenflies symbols of oriented space-group types. As you click on any of these subgroups, the Hermann–Mauguin symbol that specifies the subgroup completely appears in the lower bar of the panel, reserved for this information. Though the embellished lattice symbols used in this presentation are self-explanatory, consultation of the manual is recommended.

The option *Point* returns the lattice to its original form of the lattice of point groups.

The following is a list of tabular appendices contained in the manual:

Appendix A: correlation of various notations and Jones' faithful representation symbols;

Appendix B: Schoenflies and Hermann–Mauguin symbols of groups in standard orientations and of their subgroups;

Appendix C: isomorphisms used for defining irreducible representations;

Appendix D: standard polynomials;

Appendix E: labelling of covariants and conversion equations;

Appendix F: list of symmetry descents;

Appendix G: nonstandard lattice letters.

Our symbols for point-symmetry operations are compared with other sources in Appendix A. Symbols of all groups used in the software are given in Appendix B and isomorphisms in Appendix C. Standard polynomials in Appendix D are abbreviated symbols for more complicated polynomials that appear in the main tables. Appendix E is of primary importance for consideration of the relationship between tensor parameters and their contribution to Cartesian tensor components as already indicated in the text explaining Table 3.1.3.1. In Appendix F are listed and classified all symmetry descents considered in the main table. Consultation of Appendix G is strongly recommended to all users who want to use the lattices of equitranslational subgroups of the space groups.

3.1.7. Glossary

(a) Groups

G	point-group symmetry of the parent (prototype, high-symmetry) phase
\mathcal{G}	space-group symmetry of the parent (prototype, high-symmetry) phase

F	point-group symmetry of the ferroic (low-symmetry) phase (domain state not specified)
\mathcal{F}	space-group symmetry of the ferroic (low-symmetry) phase (domain state not specified)
F_1	point-group symmetry of the first ferroic single domain state
\mathcal{F}_1	space-group symmetry of the first ferroic single domain state
$G \Downarrow F$	point-group symmetry descent from G to F
$\mathcal{G} \Downarrow \mathcal{F}$	space-group symmetry descent from \mathcal{G} to \mathcal{F}
$\mathcal{G} \Downarrow' \mathcal{F}$	equitranslational symmetry descent from \mathcal{G} to \mathcal{F}
Γ_η	representation of \mathcal{G} (or of G) according to which η transforms
$D^{(n)}$	irreducible matrix representation of the order parameter η
χ_η	character of the matrix representation $D^{(n)}$
R -irep	physically irreducible representation
n_F	number of subgroups conjugate under G to subgroup F_1
n_f	number of ferroic single domain states
n_a	number of ferroelastic single domain states
n_e	number of ferroelectric single domain states

(b) Physical quantities

c	specific heat
$d_{i\mu}$	piezoelectric tensor
F, G	free energy
g_μ	optical activity
P_i	dielectric polarization
S	entropy
s_{ij}	elastic compliance
T_c	Curie temperature
u_{ij}, u_μ	strain tensor
V	cell volume
χ	dielectric susceptibility
ε	enantiomorphism, chirality
ε_{ij}	dielectric permittivity
η	order parameter (primary)
λ	order parameter (secondary)
ω_{LO}	longitudinal optic mode frequency
ω_{TO}	transverse optic mode frequency
$\pi_{\mu\nu}$	piezo-optic tensor

References

- Aizu, K. (1969). *Possible species of ferroelastic crystals and of simultaneously ferroelectric and ferroelastic crystals*. *J. Phys. Soc. Jpn*, **27**, 387–396.
- Aizu, K. (1970). *Possible species of ferromagnetic, ferroelectric, and ferroelastic crystals*. *Phys. Rev. B*, **2**, 754–772.
- Aizu, K. (1973). *Second order ferroic states*. *J. Phys. Soc. Jpn*, **34**, 121–128.
- Altmann, S. L. & Herzig, P. (1994). *Point-group theory tables*. Oxford: Clarendon Press.
- Aroyo, M. I. & Perez-Mato, J. M. (1998). *Symmetry mode analysis of displacive phase transitions using International Tables for Crystallography*. *Acta Cryst.* **A54**, 19–30.
- Ascher, E. (1968). *Lattices of equi-translation subgroups of the space groups*. Geneva: Battelle.
- Ascher, E. & Kobayashi, J. (1977). *Symmetry and phase transitions: the inverse Landau problem*. *J. Phys. C: Solid State Phys.* **10**, 1349–1363.