

3. PHASE TRANSITIONS, TWINNING AND DOMAIN STRUCTURES

$$\begin{aligned} N &= [G : \mathcal{F}] = [G : F][\mathbf{T} : \mathbf{U}] \\ &= (|G| : |F|)(v_{\mathcal{F}} : v_G) = (|G| : |F|)(Z_{\mathcal{F}} : Z_G) \\ &= (|G| : |F|)\det(m_{ij}) = nd_i. \end{aligned} \quad (3.2.3.91)$$

Each suborbit, represented by a row in the array (3.2.3.84), contains all basic (microscopic) domain states that are related by pure translations. These domain states exhibit the same tensor properties, *i.e.* they belong to the same ferroic domain state.

*Example [sT] 3.2.3.33.* Let us consider a phase transition with a symmetry descent  $G \supset F_1$  with an orbit  $G\mathbf{S}_{11}$  of domain states. Let  $L_1$  be an intermediate group,  $F_1 \subset L_1 \subset G$ , and  $\lambda^{(1)}$  the principal order parameter associated with the symmetry descent  $G \supset L_1$  [cf. (3.2.3.58)],  $I_G(\lambda^{(1)}) = L_1$ . Since  $L_1$  is an intermediate group, the quantity  $\lambda^{(1)}$  represents a secondary order parameter of the symmetry descent  $G \supset F_1$ . The  $G$  orbit of  $\lambda^{(1)}$  is

$$G\lambda^{(1)} = \{\lambda^{(1)}, \lambda^{(2)}, \dots, \lambda^{(m)}\}, \quad m = [G : L_1]. \quad (3.2.3.92)$$

As in Example [oT] 3.2.3.28, there is a bijection between left cosets of the decomposition of  $G$  into left cosets of  $L_1$  [see (3.2.3.80)] and the  $G$  orbit of secondary order parameters (3.2.3.92). One can, therefore, associate with the suborbit  $L_j\mathbf{S}_{j1}$  the value  $\lambda^{(j)}$  of the secondary order parameter  $\lambda$ ,

$$L_j\mathbf{S}_{j1} \leftrightarrow \lambda^{(j)}, \quad j = 1, 2, \dots, m. \quad (3.2.3.93)$$

A suborbit  $L_j\mathbf{S}_{j1}$  is thus comprised of objects of the orbit  $G\mathbf{S}_{11}$  with the same value of the secondary order parameter  $\lambda^{(j)}$ .

*Example [oS] 3.2.3.34.* Let us choose for the intermediate group  $L_1$  the normalizer  $N_G(F_1)$ . Then the suborbits equal

$$\begin{aligned} N_G(F_j)\mathbf{S}_{j1} &= \{h_j\mathbf{S}_{11}, h_j p_2\mathbf{S}_{11}, \dots, h_j p_d\mathbf{S}_{11}\}, \\ j &= 1, 2, \dots, m = [G : N_G(F_1)], \end{aligned} \quad (3.2.3.94)$$

where  $p_1 = e, p_2, \dots, p_d$  are representatives of left cosets  $p_k F_1$  in the decomposition of  $N_G(F_1)$ ,

$$N_G(F_1) = p_1 F_1 \cup p_2 F_1 \cup \dots \cup p_d F_1, \quad d = [N_G(F_1) : F_1], \quad (3.2.3.95)$$

and  $h_j$  are representatives of the decomposition (3.2.3.77). The suborbit  $F_j\mathbf{S}_{j1}$  consists of all objects with the same stabilizer  $F_j$ ,

$$\begin{aligned} I_G(\mathbf{S}_{j1}) &= I_G(\mathbf{S}_{j2}) = \dots = I_G(\mathbf{S}_{jd}) = F_j, \\ j &= 1, 2, \dots, m = [G : N_G(F_1)]. \end{aligned} \quad (3.2.3.96)$$

Propositions 3.2.3.23 and 3.2.3.30 are examples of structures that a group action induces from a group  $G$  on a  $G$ -set. Another important example is a permutation representation of the group  $G$  which associates operations of  $G$  with permutations of the objects of the orbit  $G\mathbf{S}_i$  [see *e.g.* Kerber (1991, 1999); for application of the permutation representation in domain-structure analysis and domain engineering, see *e.g.* Fuksa & Janovec (1995, 2002)].

3.2.3.3.6. Orbits of ordered pairs and double cosets

An ordered pair  $(\mathbf{S}_i, \mathbf{S}_k)$  is formed by two objects  $\mathbf{S}_i, \mathbf{S}_k$  from the orbit  $G\mathbf{S}_1$ . Let  $\mathbf{P}$  denote the set of all ordered pairs that can be formed from the objects of the orbit  $G\mathbf{S}_1$ . The group action  $\varphi$  of group  $G$  on the set  $\mathbf{P}$  is defined by the following relation:

$$\begin{aligned} \varphi : g(\mathbf{S}_i, \mathbf{S}_k) &= (g\mathbf{S}_i, g\mathbf{S}_k) = (\mathbf{S}_r, \mathbf{S}_s), \\ g &\in G, \quad (\mathbf{S}_i, \mathbf{S}_k), (\mathbf{S}_r, \mathbf{S}_s) \in \mathbf{P}. \end{aligned} \quad (3.2.3.97)$$

The requirements (3.2.3.47) to (3.2.3.49) are fulfilled, mapping (3.2.3.97) defines an action of group  $G$  on the set  $\mathbf{P}$ .

The group action (3.2.3.97) introduces the  $G$ -equivalence of ordered pairs: Two ordered pairs  $(\mathbf{S}_i, \mathbf{S}_k)$  and  $(\mathbf{S}_r, \mathbf{S}_s)$  are crystallographically equivalent (with respect to the group  $G$ ),  $(\mathbf{S}_i, \mathbf{S}_k) \stackrel{G}{\sim} (\mathbf{S}_r, \mathbf{S}_s)$ , if there exists an operation  $g \in G$  that transforms  $(\mathbf{S}_i, \mathbf{S}_k)$  into  $(\mathbf{S}_r, \mathbf{S}_s)$ ,

$$g \in G \quad (g\mathbf{S}_i, g\mathbf{S}_k) = (\mathbf{S}_r, \mathbf{S}_s), \quad (\mathbf{S}_i, \mathbf{S}_k), (\mathbf{S}_r, \mathbf{S}_s) \in \mathbf{P}. \quad (3.2.3.98)$$

An orbit of ordered pairs  $G(\mathbf{S}_i, \mathbf{S}_k)$  comprises all ordered pairs crystallographically equivalent with  $(\mathbf{S}_i, \mathbf{S}_k)$ . One can choose as a representative of the orbit  $G(\mathbf{S}_i, \mathbf{S}_k)$  an ordered pair  $(\mathbf{S}_1, \mathbf{S}_j)$  with the first member  $\mathbf{S}_1$  since there is always an operation  $g_{i1} \in G$  such that  $g_{i1}\mathbf{S}_i = \mathbf{S}_1$ . The orbit  $F_1(\mathbf{S}_1, \mathbf{S}_j)$  assembles all ordered pairs with the first member  $\mathbf{S}_1$ . This orbit can be expressed as

$$\begin{aligned} F_1(\mathbf{S}_1, \mathbf{S}_j) &= (F_1\mathbf{S}_1, F_1\mathbf{S}_j) = (\mathbf{S}_1, F_1(g_j\mathbf{S}_1)) \\ &= (\mathbf{S}_1, (F_1g_j)(F_1\mathbf{S}_1)) = (\mathbf{S}_1, (F_1g_jF_1)\mathbf{S}_1), \end{aligned} \quad (3.2.3.99)$$

where the identity  $F_1\mathbf{S}_1 = \mathbf{S}_1$  [see relation (3.2.3.70)] has been used.

Thus the double coset  $F_1g_jF_1$  contains all operations from  $G$  that produce all ordered pairs with the first member  $\mathbf{S}_1$  that are  $G$ -equivalent with  $(\mathbf{S}_1, \mathbf{S}_j = g_j\mathbf{S}_1)$ . If one chooses  $g_r \in G$  that is not contained in the double coset  $F_1g_jF_1$ , then the ordered pair  $(\mathbf{S}_1, \mathbf{S}_r = g_r\mathbf{S}_1)$  must belong to another orbit  $G(\mathbf{S}_1, \mathbf{S}_r) \neq G(\mathbf{S}_1, \mathbf{S}_j)$ . Hence to distinct double cosets there correspond distinct classes of ordered pairs with the first member  $\mathbf{S}_1$ , *i.e.* distinct orbits of ordered pairs. Since the group  $G$  can be decomposed into disjoint double cosets [see (3.2.3.36)], one gets

*Proposition 3.2.3.35.* Let  $G$  be a group and  $\mathbf{P}$  a set of all ordered pairs that can be formed from the objects of the orbit  $G\mathbf{S}_1$ . There is a one-to-one correspondence between the  $G$  orbits of ordered pairs of the set  $\mathbf{P}$  and the double cosets of the decomposition

$$G = F_1 \cup F_1g_2F_1 \cup \dots \cup F_1g_jF_1 \cup \dots \cup F_1g_qF_1, \quad j = 1, 2, \dots, q. \quad (3.2.3.100)$$

$$G(\mathbf{S}_1, \mathbf{S}_j) \leftrightarrow F_1g_jF_1 \quad \text{where } \mathbf{S}_j = g_j\mathbf{S}_1. \quad (3.2.3.101)$$

This bijection allows one to express the partition of the set  $\mathbf{P}$  of all ordered pairs into  $G$  orbits,

$$\mathbf{P} = G(\mathbf{S}_1, \mathbf{S}_1) \cup G(\mathbf{S}_1, g_2\mathbf{S}_1) \cup \dots \cup (\mathbf{S}_1, \mathbf{S}_j) \cup \dots \cup G(\mathbf{S}_1, g_q\mathbf{S}_1), \quad (3.2.3.102)$$

where  $\{g_1 = e, g_2, \dots, g_j, \dots, g_q\}$  is the set of representatives of double cosets in the decomposition (3.2.3.100) (Janovec, 1972).

Proposition 3.2.3.35 applies directly to pairs of domain states (domain pairs) and allows one to find transposition laws that can appear in the low-symmetry phase (see Section 3.4.3).

For more details and other applications of group action see *e.g.* Kopský (1983), Lang (1965), Michel (1980), Opechowski (1986), Robinson (1982), and especially Kerber (1991, 1999).

References

Aizu, K. (1969). Possible species of "ferroelastic" crystals and of simultaneously ferroelectric and ferroelastic crystals. *J. Phys. Soc. Jpn*, **27**, 387–396.

### 3.2. TWINNING AND DOMAIN STRUCTURES

- Aizu, K. (1970). *Possible species of ferromagnetic, ferroelectric and ferroelastic crystals*. *Phys. Rev. B*, **2**, 754–772.
- Aizu, K. (1972). *Electrical, mechanical and electromechanical orders of state shifts in nonmagnetic ferroic crystals*. *J. Phys. Soc. Jpn*, **32**, 1287–1301.
- Blattner, H., Känzig, W., Merz, W. & Sutter, H. (1948). *Die Domänenstruktur von BaTiO<sub>3</sub>-Kristallen*. *Helv. Phys. Acta*, **21**, 207–209.
- Bloss, F. D. (1971). *Crystallography and crystal chemistry*, pp. 324–338. New York: Holt, Rinehart and Winston.
- Bollmann, W. (1970). *Crystal defects and crystalline interfaces*, ch. 12, pp. 143–148. Berlin: Springer.
- Bollmann, W. (1982). *Crystal lattices, interfaces, matrices*, pp. 111–249. Geneva: published by the author.
- Bradley, C. J. & Cracknell, A. P. (1972). *The mathematical theory of symmetry in solids*. Oxford: Clarendon Press.
- Budden, F. J. (1972). *Fascination of groups*. Cambridge University Press.
- Buerger, M. J. (1945). *The genesis of twin crystals*. *Am. Mineral.* **30**, 469–482.
- Cady, W. G. (1946). *Piezoelectricity*, ch. XXV. New York: McGraw-Hill.
- Cahn, R. W. (1954). *Twinned crystals*. *Adv. Phys.* **3**, 202–445.
- Chernysheva, M. A. (1950). *Mechanical twinning in crystals of Rochelle salt*. *Dokl. Akad. Nauk SSSR*, **74**, 247–249. (In Russian.)
- Donnay, G. & Donnay, J. D. H. (1974). *Classification of triperiodic twins*. *Can. Mineral.* **12**, 422–425.
- Donnay, J. D. H. (1940). *Width of albite-twinning lamellae*. *Am. Mineral.* **25**, 578–586.
- Donnay, J. D. H. & Donnay, G. (1972). *Crystal geometry*. In *International Tables for X-ray Crystallography*, Vol. II, 2nd edition, edited by J. C. Kasper & K. Lonsdale, Section 3. Birmingham: Kynoch Press.
- Fischmeister, H. F. (1985). *Structure and properties of high angle grain boundaries*. *J. Phys. (Paris)*, **46**, Suppl. C4-3–23.
- Friedel, G. (1904). *Etude sur les groupements cristallins*. *Extrait du Bulletin de la Société d'Industrie Minérale*, Quatrième Série, Tomes III et IV. Saint Etienne: Imprimerie Théolier J. et Cie.
- Friedel, G. (1926). *Leçons de cristallographie*. Nancy, Paris, Strasbourg: Berger-Levrault. [Reprinted (1964). Paris: Blanchard.]
- Fuksa, J. & Janovec, V. (1995). *Permutation classification of domain pairs*. *Ferroelectrics*, **172**, 343–350.
- Fuksa, J. & Janovec, V. (2002). *Macroscopic symmetries and domain configurations of engineered domain structures*. *J. Phys. Condens. Matter*, **14**, 3795–3812.
- Giacovazzo, C. (1992). Editor. *Fundamentals of crystallography*, pp. 80–87, 133–140. Oxford University Press.
- Gottstein, G. & Shvindlerman, L. S. (1999). *Grain boundary migration in metals*, ch. 2. London: CRC Press.
- Hahn, Th., Janovec, V. & Klapper, H. (1999). *Bicrystals, twins and domain structures – a comparison*. *Ferroelectrics*, **222**, 11–21.
- Hahn, Th. & Wondratschek, H. (1994). *Symmetry of crystals*. Sofia: Heron Press Ltd.
- Hall, M. Jr (1959). *The theory of groups*. New York: The Macmillan Company.
- Hámos, L. von & Thiessen, P. A. (1931). *Über die Sichtbarmachung von Bezirken verschiedenen ferromagnetischen Zustandes fester Körper*. *Z. Phys.* **71**, 442–444.
- Haüy, R.-J. (1801). *Traité de minéralogie I*, p. 273. Paris: Delance.
- Indenbom, V. L. (1960). *Phase transitions without change in the number of atoms in the unit cell of the crystal*. *Sov. Phys. Crystallogr.* **5**, 106–115.
- International Tables for Crystallography* (2002). Vol. A. *Space-group symmetry*, 5th edition, edited by Th. Hahn. Dordrecht: Kluwer Academic Publishers.
- International Tables for Crystallography* (2003). Vol. A1. *Symmetry relations between space groups*, edited by H. Wondratschek & U. Müller. In preparation.
- Janovec, V. (1972). *Group analysis of domains and domain pairs*. *Czech. J. Phys. B*, **22**, 974–994.
- Janssen, T. (1973). *Crystallographic groups*. Amsterdam: North-Holland.
- Kalonji, G. (1985). *A roadmap for the use of interfacial symmetry groups*. *J. Phys. (Paris) Colloq.* **46**, C4-249–255.
- Kay, H. F. (1948). *Preparation and properties of crystals of barium titanate, BaTiO<sub>3</sub>*. *Acta Cryst.* **1**, 229–237.
- Kerber, A. (1991). *Algebraic combinatorics via finite group action*. Mannheim: B. I. Wissenschaftsverlag.
- Kerber, A. (1999). *Applied finite group actions*. Berlin: Springer.
- Klassen-Neklyudova, M. V. (1964). *Mechanical twinning of crystals*. New York: Consultants Bureau.
- Klassen-Neklyudova, M. V., Chernysheva, M. A. & Shternberg, A. A. (1948). *The real structure of crystals of Rochelle salt*. *Dokl. Akad. Nauk SSSR*, **63**, 527–530. (In Russian.)
- Klein, C. (1869). *Zwillingsverbindungen und Verzerrungen*. Heidelberg: G. Mohr.
- Koch, E. (1999). *Twinning*. In *International tables for crystallography*, Vol. C. *Mathematical, physical and chemical tables*, 2nd edition, edited by A. J. C. Wilson & E. Prince, Section 1.3. Dordrecht: Kluwer Academic Publishers.
- Kopský, V. (1983). *Algebraic investigations in Landau model of structural phase transitions, I, II, III*. *Czech. J. Phys. B*, **33**, 485–509, 720–744, 845–869.
- Kuratowski, K. & Mostowski, A. (1968). *Set theory*. Amsterdam: North-Holland.
- Landau, L. D. (1937). *On the theory of phase transitions. I and II*. *Zh. Eksp. Teor. Fiz.* **7**, pp. 19, 627 (in Russian); *Phys. Z. Sowjet.* **11**, pp. 26, 545 (in German). *Collected papers of L. D. Landau*, edited by D. Ter Haar (1967). New York: Gordon and Breach.
- Lang, S. (1965). *Algebra*. Reading, MA: Addison-Wesley.
- Ledermann, W. (1973). *Introduction to group theory*. London: Longman Group Ltd.
- Lipschutz, S. (1981). *Theory and problems of set theory and related topics*. Singapore: McGraw-Hill.
- Mallard, E. (1879). *Traité de cristallographie, géométrie et physique*. Vol. I. Paris: Dunod.
- Matthias, B. & von Hippel, A. (1948). *Domain structure and dielectric response of barium titanate single crystals*. *Phys. Rev.* **73**, 1378–1384.
- Michel, L. (1980). *Symmetry defects and broken symmetry. Configurations. Hidden symmetry*. *Rev. Mod. Phys.* **52**, 617–651.
- Mohs, F. (1822, 1824). *Grundriss der Mineralogie*, two volumes. Dresden: Arnold. [English translation by Haidinger, W. (1825): *Treatise on mineralogy*, three volumes. Edinburgh: Constable.]
- Mohs, F. (1823). *On the crystallographic discoveries and systems of Mohs and Weiss*. *Edinburgh Philos. J.* **8**, 275–290.
- Mueller, H. (1935). *Properties of Rochelle salt*. *Phys. Rev.* **47**, 175–191.
- Naumann, C. F. (1830). *Lehrbuch der reinen und angewandten Krystallographie*. Vol. II, p. 203. Leipzig: Brockhaus.
- Naumann, C. F. (1856). *Elemente der theoretischen Krystallographie*. p. 67. Leipzig: W. Engelmann.
- Niggli, P. (1919). *Geometrische Krystallographie des Diskontinuums*. Leipzig: Borntraeger. [Reprinted (1973). Wiesbaden: Sändig.]
- Niggli, P. (1920, 1924, 1941). *Lehrbuch der Mineralogie und Kristallchemie*, 1st ed. 1920, 2nd ed. 1924, 3rd ed., Part I, 1941, pp. 136–153, 401–414. Berlin-Zehlendorf: Gebrüder Borntraeger.
- Opechowski, W. (1986). *Crystallographic and metacrystallographic groups*. Amsterdam: North-Holland.
- Pond, R. C. & Bollmann, W. (1979). *The symmetry and interfacial structure of bicrystals*. *Philos. Trans. R. Soc. London Ser. A*, **292**, 449–472.
- Pond, R. C. & Vlachavas, D. S. (1983). *Bicrystallography*. *Proc. R. Soc. London Ser. A*, **386**, 95–143.
- Robinson, D. J. S. (1982). *A course in the theory of groups*. New York: Springer.
- Romé de l'Isle, J. B. L. (1783). *Cristallographie*. Vol. I, 2nd edition, p. 93. Paris: Imprimerie de Monsieur.
- Rosen, J. (1995). *Symmetry in science*. Berlin: Springer.
- Shubnikov, A. V. & Koptsik, V. A. (1974). *Symmetry in science and art*, pp. 348, 372. New York: Plenum.
- Speiser, A. (1927). *Theorie der Gruppen von endlicher Ordnung*. Berlin: Springer.
- Sutton, A. P. & Balluffi, R. W. (1995). *Interfaces in crystalline materials*, Section 1.5, pp. 25–41. Oxford: Clarendon Press.
- Tertsch, H. (1936). *Bemerkungen zur Frage der Verbreitung und zur Geometrie der Zwillingsbildungen*. *Z. Kristallogr.* **94**, 461–490.
- Tschermak, G. (1904). *Einheitliche Ableitung der Kristallisations- und Zwillingsgesetze*. *Z. Kristallogr.* **39**, 433–462.
- Tschermak, G. (1906). *Lehrbuch der Mineralogie*. Wien: Hölder.
- Tschermak, G. & Becke, F. (1915). *Lehrbuch der Mineralogie*. 7th edition, pp. 93–114. Wien: Hölder.
- Vainshtein, B. K. (1994). *Modern crystallography I. Symmetry of crystals*, 2nd edition. Berlin: Springer.

### 3. PHASE TRANSITIONS, TWINNING AND DOMAIN STRUCTURES

- Vainshtein, B. K., Fridkin, V. M. & Indenbom, V. L. (1995). *Modern crystallography II. Structure of crystals*, 2nd edition, Section 5.7. Berlin: Springer.
- Valasek, J. (1921). *Piezoelectricity and allied phenomena in Rochelle salt*. *Phys. Rev.* **17**, 475–481.
- Van Tendeloo, G. & Amelinckx, S. (1974). *Group-theoretical considerations concerning domain formation in ordered alloys*. *Acta Cryst.* **A30**, 431–440.
- Wadhawan, V. K. (1997). *A tensor classification of twinning in crystals*. *Acta Cryst.* **A53**, 546–555.
- Wadhawan, V. K. (2000). *Introduction to ferroic materials*. Amsterdam: Gordon and Breach.
- Weiss, Chr. S. (1809). *De Indagando Formarum Crystallinarum Characteres Geometrico Principali*. Dissertatio. Leipzig: Tauchnitz. [French translation by Brochant de Villiers, A. (1811): *Mémoire sur la détermination du caractère géométrique principal des formes cristallines*. *J. Mines*, **29**, 349–391, 401–444.]
- Weiss, Chr. S. (1814). *Schweigers Journal für Physik und Chemie*, Vol. X, p. 223.
- Weiss, Chr. S. (1817, 1818). *Magazin der Gesellschaft naturforschender Freunde zu Berlin*, Vol. VII, p. 183, Vol. VIII, p. 27.
- Weiss, P. (1907). *L'hypothèse du champ moléculaire et la propriété ferromagnétique*. *J. Phys. Radium*, **6**, 661–690.
- Wondratschek, H. (1995). *Splitting of Wyckoff positions (orbits)*. *Z. Kristallogr.* **210**, 567–573.
- Wondratschek, H. & Aroyo, M. (2001). *The application of Hermann's group  $\mathcal{M}$  in group-subgroup relations between space groups*. *Acta Cryst.* **A57**, 311–320.
- Zheludev, I. S. & Shuvalov, L. A. (1956). *Seignettelectric phase transitions and crystal symmetry*. *Kristallografiya*, **1**, 681–688. (In Russian.) [English translation: *Sov. Phys. Crystallogr.* **1**, 537–542].
- Zwicker, B. & Scherrer, P. (1944). *Elektrooptische Eigenschaften der seignette-elektrischen Kristalle  $KH_2PO_4$  und  $KD_2PO_4$* . *Helv. Phys. Acta*, **17**, 346–373.