3.1. STRUCTURAL PHASE TRANSITIONS

(La) below the symbol of the irreducible representation Γ_η indicates that the *Landau condition* is violated, hence the transition cannot be continuous (second order). The Landau condition requires the absence of the third-degree invariant polynomial of the order-parameter components (the symmetrized triple product $[\Gamma_\eta]^3$ must not contain the identity representation of G). For more details see Lyubarskii (1960), Kociński (1983, 1990), Tolédano & Tolédano (1987), Izyumov & Syromiatnikov (1990) and Tolédano & Dmitriev (1996).

(Li) below the symbol of the irreducible representation Γ_η means that the *Lifshitz condition* is violated, hence the transition to a homogeneous ferroic phase is not continuous. The Lifshitz condition demands the absence of invariant terms that couple bilinearly the order-parameter components with their spatial derivatives that are not exact differentials (the antisymmetric square $\{\Gamma_\eta\}^2$ has no representation in common with the vector representation of G). For more details see Lyubarskii (1960), Kociński (1983, 1990), Tolédano & Tolédano (1987), Izyumov & Syromiatnikov (1990) and Tolédano & Dmitriev (1996).

If there is no symbol (La) and/or (Li) below the symbol of the R-irep Γ_η (*i.e.* if both Landau and Lifshitz conditions are fulfilled), then the R-irep is called an *active representation*. In the opposite case, the R-irep is a *passive representation* (Lyubarskii, 1960; Kociński, 1983, 1990).

Standard variables: components of the order parameter in the carrier space of the irreducible representation Γ_η expressed in so-called *standard variables* (see the manual of the software *GI⋆KoBo*-1). Upper and lower indices and the typeface of standard variables allow one to identify to which irreducible representation Γ_η they belong. Standard variables of one-dimensional representations are denoted by x (Sans Serif typeface), two- or three-dimensional R-ireps by x, y or x, y, z, respectively. Upper indices $^+$ and $^-$ correspond to the lower indices g (*gerade*) and u (*ungerade*) of spectroscopic notation, respectively. The lower index specifies to which irreducible representation the variable belongs.

For multidimensional representations, a general vector of the carrier space V_η is given in the last row; this vector is invariant under the kernel of Γ_η that appears as a low-symmetry group in column F_1. The other rows contain special vectors defined by equal or zero values of some standard variables; these vectors are invariant under epikernels of Γ_η given in column F_1.

F_1: short international (Hermann–Mauguin) and Schoenflies symbol of the point group F_1 which describes the symmetry of the first single domain state of the ferroic (low-symmetry) phase. The subscripts define the orientation of symmetry elements (generators) of F_1 in the Cartesian crystallophysical coordinate system of the group G (see Figs. 3.4.2.3 and 3.4.2.4, and Tables 3.4.2.5 and 3.4.2.6). This specifies the orientation of the group F_1, which is a prerequisite for domain structure analysis (see Chapter 3.4).

n_F: number of subgroups conjugate to F_1 under G. If $n_F = 1$, the group F_1 is a normal subgroup of G (see Section 3.2.3).

Principal tensor parameters: covariant tensor components, *i.e.* linear combinations of Cartesian tensor components that transform according to the same matrix R-irep $D^{(\eta)}$ as the primary order parameter η. Principal tensor parameters are given in this form in the software *GI⋆KoBo*-1 and in Kopský (2001).

This presentation is in certain situations not practical, since property tensors are usually described by numerical values of their Cartesian components. Then it is important to know morphic Cartesian tensor components and symmetry-breaking increments of nonzero Cartesian components that appear spontaneously in the ferroic phase. The bridge between these two presentations is
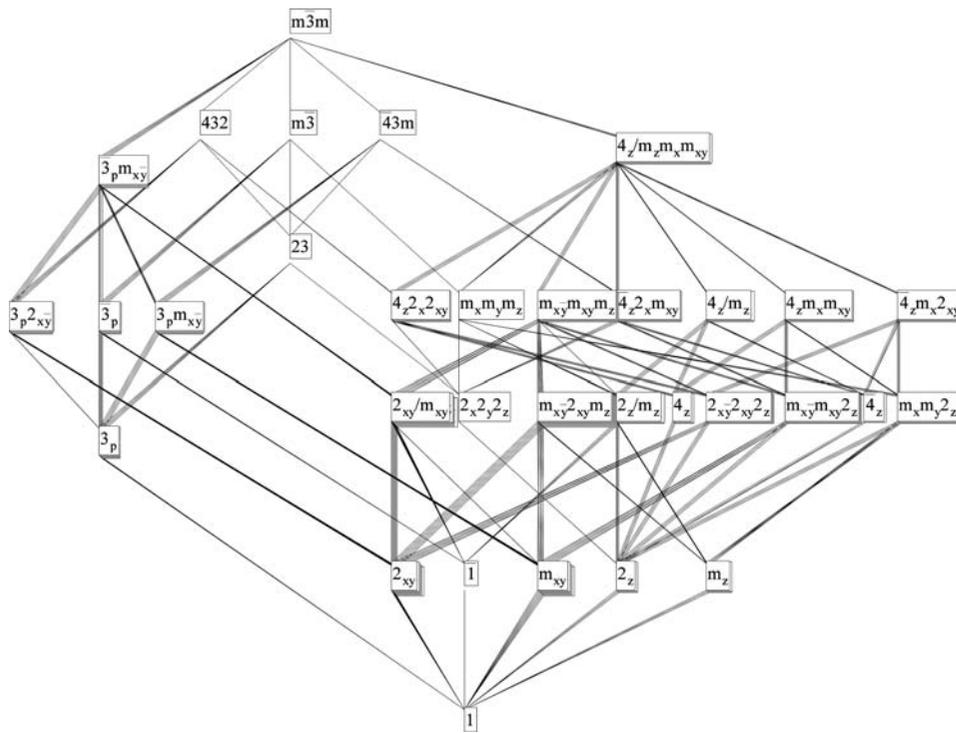

Fig. 3.1.3.1. Lattice of subgroups of the group $m\bar{3}m$. Conjugate subgroups are depicted as a pile of cards. In the software *GI⋆KoBo*-1, one can pull out individual conjugate subgroups by clicking on the pile.
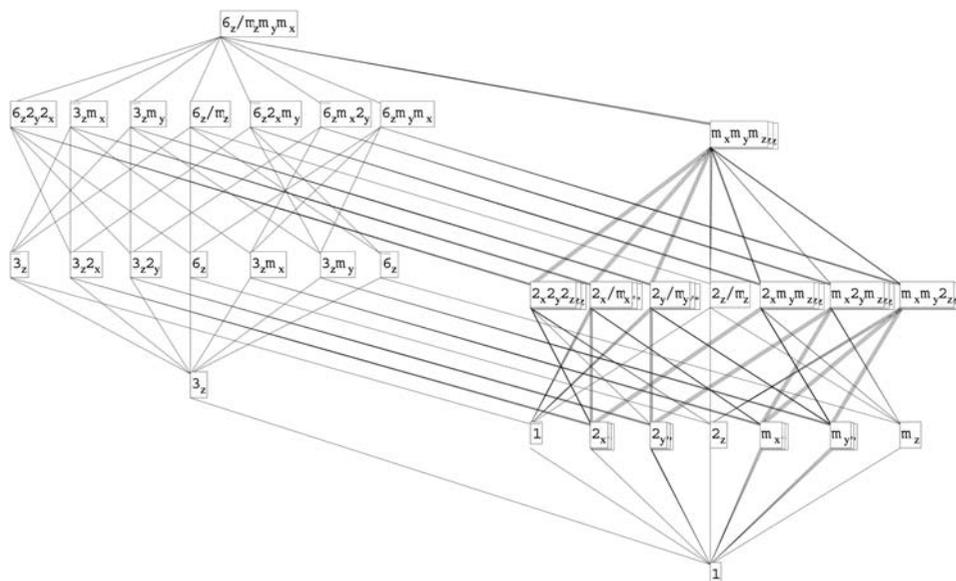

Fig. 3.1.3.2. Lattice of subgroups of the group $6/mmm$. Conjugate subgroups are depicted as a pile of cards. In the software *GI⋆KoBo*-1, one can pull out individual conjugate subgroups by clicking on the pile.

references