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computer program abstracts

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INVARIANTS: program for obtaining a list of invariant polynomials of the order-parameter components associated with irreducible representations of a space group

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1. The crystallographic problem

In a crystalline phase transition, the space-group symmetry of the high- and low-symmetry phases often exhibits a group–subgroup relationship: $L \subset H$. In the Landau theory of phase transitions, this transition is described by a primary order parameter (OP). Such an OP is an n-dimensional vector $\boldsymbol{\eta}$ in the space defined by an irreducible representation (IR) of H. The action of the symmetry transformations induces corresponding transformations on the basis of the IR. The most general invariant free energy Φ ('Landau potential'), which describes the energy change at the transition, is expressed as homogeneous sets of polynomials of the OP components of degree p, each polynomial being invariant under the symmetry group H. The high-symmetry group H corresponds to $\boldsymbol{\eta} = 0$ and the low-symmetry group L to the minimum of Φ for non-zero $\boldsymbol{\eta}$. In addition to the primary OP there are also secondary OPs which correspond to other IRs of H and which couple to the primary OP. These secondary OPs also play a role in the transition as additional distortions and thus invariants corresponding to these IRs, along with their coupling with the primary OP, are of interest. The aim of the program is to generate symmetry-allowed invariants associated with a given high-symmetry group H and the primary OP, along with invariants and coupling polynomials of the secondary OPs.

2. Method of solution

Given a set of OPs (primary and secondary), we form a reducible representation Γ of H which is a direct sum of the irreducible representations corresponding to the OPs. The representation Γ maps symmetry operations $h \in H$ onto N-dimensional matrices $D(h)$. We form a composite OP $\boldsymbol{\eta}$ which is an N-dimensional vector containing the components of all of the primary and secondary OPs. A symmetry operation h in Γ is just ordinary matrix multiplication on the components of $\boldsymbol{\eta}$, *i.e.* $h\boldsymbol{\eta}$ means $D(h)\boldsymbol{\eta}$. We generate invariant polynomials by projecting them out from an arbitrary monomial $P_0(\boldsymbol{\eta})$, *i.e.* $P(\boldsymbol{\eta}) = \sum_h P_0(h\boldsymbol{\eta})$, where the sum is over all operators h which are mapped onto distinct matrices $D(h)$. By trying all possible monomials $P_0(\boldsymbol{\eta})$ of pth degree, we obtain all possible invariant polynomials $P(\boldsymbol{\eta})$ of that degree. We use the characters of the pth-degree symmetric direct product to calculate the number of independent invariant polynomials of that degree (see Lyubarskii, 1960), so that we can know when we are finished. The form of the invariant polynomials generally depends on the choice of matrices $D(h)$. The specific matrix representations used are those given by Stokes & Hatch (1988).

3. Software environment

INVARIANTS is written in Fortran 90 and has been implemented under the Linux operating system.

4. Program specification

Input:

(i) A space group of the high-symmetry group H is chosen from a drop-down list showing the space-group numbers and symbols from *International Tables for Crystallography* (1995).

(ii) The **k** point for the IR is chosen from a drop-down list. If needed, parameter values for the **k** points are also entered. The coordinates for the points in the first Brillouin zone are given as well as the symbols from Miller & Love (1967) and Kovalev (1993).

(iii) The IR is chosen from a drop-down list.

(iv) The direction for the OP is chosen from a drop-down list.

(v) The further selection of the OP is chosen from a drop-down list of symmetry equivalent OP forms.

(vi) Additional OPs from different IRs can be selected if coupled OPs are to be considered.

(vii) The range of polynomial degree is chosen.

Output:

The information used as input above is shown and the invariants of each degree, within the range chosen by the user, along with the IRs, are given. The calculation may require a few minutes for some cases with many degrees of freedom. We have restricted the list of order-parameter directions to those with no more than eight degrees of freedom.

5. Documentation and availability

The program can be run over the Internet using any computer with an Internet browser. The URL of the program is http://www.physics.byu.edu/~stokesh/invariants.html. Running the program requires no local installation. Documentation (including an example) is available at this URL. Furthermore, a more complete discussion of the role of invariants, including example polynomial forms, can be found in works by Stokes & Hatch (1988, 1991) and Saxena *et al.* (1994).

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