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Remarks on the Classification of Crystal Lattices

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Results are sketched which were obtained while attempting to understand some classical concepts of crystallography of lattices, in view of presenting a nonstandard viewpoint on the invariance of continuum constitutive equations for thermoelastic crystals capable of undergoing phase transitions and related phenomena like twinning and microstructure formation.

Discussion of the results

G. Zanzotto and I have been involved for some time now in the development of a thermoelastic model for crystalline solids that overcomes the limitations of standard elastic theories, in particular regarding invariance requirements. This research has originated from works of Ericksen (1970, 1977, 1979, 1980/1, 1980/2) and Parry (1976, 1978, 1980) and has considerably progressed in these years, in various directions, involving a largely interdisciplinary community of researchers.

Molecular models of elasticity, of the kind proposed by Born (1915) based on early work of Cauchy (1828/1, 1828/2, 1829) are important for motivating the invariance assumptions in the aforementioned model of crystal elasticity. Therefore, in trying to write an organized presentation of the model for newcomers, we also had to revisit some of the classical notions and theorems of crystallography.

While the classification of crystallographic point group, based on orthogonal conjugacy, is well presented in most references on crystallography (see for instance Senechal (1990)), the classification of crystal lattices is not at all so.[1] In most cases one is only informed, with no justification, that these can be divided into 14 classes, representatives of which are given in a figure, grouped into crystal systems, within each one of which they differ by the centering. So, for instance, lattices of cubic symmetry can be of either primitive cubic, or face-centered cubic or body-centered cubic type. The names are almost self-explanatory.

In a few references, for instance Opechowski (1986), the 14 Bravais lattices, or types of lattices, come out as a corollary of the classification of crystallographic space groups, which is based on group isomorphism, or equivalently on conjugacy within the group of affine transformations by a renowned theorem of Bieberbach (1912). Although here the classification criterion is spelled out, it is based on results obtained at the turn of 20th century, some 50 years after the celebrated paper (Bravais, 1850) in which Bravais analyzes lattices and produces the 14 (classes or) types. So, the space-group criterion could hardly have been the one adopted by Bravais, and perhaps the same could be said of the *arithmetic criterion*: two lattices are of the same type if their symmetry groups have the same representation in suitable respective *lattice bases* (see footnote 1 for a comparison with the geometric criterion). The arithmetic criterion, based on result on the arithmetic classification of quadratic forms, mainly due to Seeber (1831), Jordan (1880), Sohncke (1874) and Frobenius (1911), besides Bieberbach, were exploited in the early 1900s (see Burckhard (1947), Niggli and Novacki (1935)), to show that there are exactly 14 arithmetic classes of three-dimensional lattices.

Bravais (1850) himself testifies that the problem of deciding when two lattices are of the 'same type' is a nontrivial one, by acknowledging 'the beautiful research work' of Frankenheim (1842), in fact leading to 15 classes, and then correcting him by showing that two classes of his in the monoclinic system actually coincide.

Setting apart constructions based on the space-group or the arithmetic classification, we only found in Miller (1972) (and later in Sternberg (1994)) an explicit construction of the 14 Bravais lattices, but no classification criterion spelled out.

[1] According to the *geometric criterion*, based on point-group symmetry, two lattices are of the same type if their point groups have the same representation in suitable respective orthonormal bases. This leads to the seven *crystal systems*.

Turning then to Bravais' own paper, we discovered the following:

1 the construction given by Miller (and Sternberg) is in fact Bravais';

2 after the 14 classes are constructed, Bravais states his criterion: two simple lattices in the same crystal system belong to the same lattice type if and only if there is a continuous deformation that brings the first lattice onto the second one without ever loosing symmetry elements.

The criterion stated is particularly interesting for a student of mechanics, with possible implications in the analysis of phase transitions; and reveals the interaction of Bravais with Cauchy, who was working on molecular models of elasticity, and actually presented Bravais' paper to the Academy.

The criterion stated by Bravais is not apparently used by himself in his construction of the 14 classes. Also, the condition of not loosing symmetry elements along the deformation path has to be interpreted as never having along it a point group in a system strictly 'contained' in the one of the initial and final configurations. A detailed discussion is given in Pitteri and Zanzotto (1996). There one also finds an explicit and exhaustive analysis of the classification based on Bravais' criterion, which actually produces 11, and not 14 classes. Indeed, three pairs of types, one in the monoclinic and two in the orthorhombic system, are distinct in Bravais' construction (and are indeed distinct according to the arithmetic criterion), but can be connected by a continuous deformation along which the point group always belongs to the monoclinic [orthorhombic] system, except one configuration where it 'increases' to orthorhombic [tetragonal].

Our conclusion is that the criterion spelled out by Bravais is very interesting, but does not seem to lead to the 14 classes that he regards as distinct. This result is obtained by means of the arithmetic criterion, which we regard as fundamental in the description of symmetry of crystalline solids. And, in this respect, Bravais was after all right.

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