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Semi-defects

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Résumé. — Nous introduisons le concept de semi-défaut pour des milieux ordonnés, où le paramètre d'ordre se divise en deux composantes couplées. Une singularité est un semi-défaut si elle est singulière pour une des composantes et continue pour l'autre. Une théorie topologique des semi-défauts est présentée. Les défauts d'empilement, qui ne sont pas encore pris en compte par la classification topologique, se révèlent être des formes particulières de semi-défauts.

Abstract. — The notion of semi-defect is introduced for ordered media, where the order parameter divides into two coupled components. A singularity is a semi-defect, if it is singular in only one of the components, and continuous in the other. A topological theory of semi-defects is presented. Stacking faults, hitherto not comprised by the topological defect classification, are special forms of semi-defects.

1. Introduction.

For a topological classification of defects in ordered media, it suffices to consider the type of order parameter (phase, unit vector, or orthogonal tripod, for example), and to determine the connectivity properties of the corresponding order parameter space (circle, sphere, $SO(3)$) [1, 2]. These properties are expressed by homotopy groups, which at once render the classes of point, line, or wall singularities. Frequently, however, the order parameter displays a substructure : in a smectic A liquid crystal, for instance, one finds positional order of the molecules in the form of layers, and orientational order in the form of a director field. Both orders are strongly coupled by the condition, that the directors stand perpendicular to the layers. In the order parameter of a biaxial nematic liquid crystal, one can clearly distinguish a (« long ») main axis from (« short ») bi-axes, orthogonal to each other. Another example is provided by the structure of those metal alloys which consists of a basic lattice and a superlattice. The two lattice constants are related by a rational number. In this Letter we will demonstrate that the fine structure of the order parameter space gives rise to new types of defects, which we denote as « semi-defects ».

2. Examples and definition of semi-defects.

Figure 1a shows a 180° -disclination both in the director order and in the layer order of a smectic A liquid crystal. In contrast, the edge dislocation of figure 1b is a semi-defect, because it is singular only in one, the layer order (the phase of the mass density wave), whereas the director field remains continuous. Any disclination of a biaxial nematic liquid crystal, where the field of the long axes is continuous, represents a semi-defect. When the main axis is fixed, the remaining degree of freedom is a planar angle (modulo π). Therefore the classes of semi-defects are the same as the classes of defects of a plane director [3] and are labelled by half-integer winding numbers. The singular wall in the alloy of figure 2 is a semi-defect, since only the superlattice is perturbed, not the sublattice. From these examples, we can draw the following definition : given an order parameter (in this Letter termed as the full order parameter), which divides into two coupled components, say component 1 and 2, a semi-defect is the region where the field of component 1 is continuous, that of component 2 discontinuous [4].

In contrast to a conventional topologically stable defect, some types of semi-defects can terminate in the bulk of an ordered medium, similarly as the Dirac string of magnetic flux ends at a magnetic monopole. The boundary of a d -dimensional semi-defect is a singularity of dimension $(d - 1)$ in component 1 of the order parameter. The singular wall of the superlattice of figure 2, for example, is bounded by two dislocation lines of the sublattice.

Fig. 1. — Singularities in smectic A liquid crystals. (a) 180° -disclination, representing a « full » defect : both the order of the layers and the order of the directors contain a singular line. (b) Edge dislocation in the order of the layers, representing a semi-defect : the director field remains continuous.

Fig. 2. — Wall defect in the superlattice of an alloy perpendicular to the paper plane. The sublattice is undisturbed. The semi-defect wall is bounded by two partial dislocations.

When considered as « full » defects, semi-defects can be unstable, i.e. if one applies the conventional description of the uniform medium by one — the complete — order parameter, they can belong to the class of topologically unstable singularities. A 4π -disclination is a stable defect of a plane director (of winding number 2), and therefore represents a stable semi-defect of biaxial nematic liquid crystals. But if viewed as a system of only one, namely the biaxial order, the 4π -disclination can vanish. A closer investigation reveals, that in the relaxation process of the 4π -disclination to the non-singular state a singularity in the main axes has to appear intermediately. It forms an energy barrier, over which the system has to climb and provides the stability for the semi-defect.

Semi-defects can be generated in a phase transition by defects in component 1 of the order parameter. The singular wall of figure 2 grows out of a dislocation of the basic lattice, when the superlattice develops at the transition point [5].

3. Topological classification of semi-defects : special case.

We denote by G an unbroken symmetry group of the medium, by $H_2 \subset G$ the symmetry group of the full order parameter, and by $H_1 \subset G$ the symmetry group of component 1 of the order parameter. As a special case we assume $H_2 \subset H_1$, as it is found in all the examples mentioned; thus the symmetry is broken in two steps from G to H_2 . Since component 1 of the order parameter is continuous around the semi-defect, locally it can be deformed into a constant field of symmetry H_1 . Then, in a neighbourhood of the semi-defect, the total order parameter is restricted to the subspace H_1/H_2 of the order parameter space G/H_2 . In n spatial dimensions, the semi-defect of dimension d is labelled by an element of the homotopy group $\pi_r(H_1/H_2)$, $r = n - d - 1$ [6]. Defects in component 1 of the order parameter, semi-defects, and defects in the full order are related by the exact sequence of homotopy groups [5, 7].

$$\cdots \rightarrow \pi_{r+1}(G/H_1) \xrightarrow{\partial} \pi_r(H_1/H_2) \xrightarrow{i} \pi_r(G/H_2) \rightarrow \cdots \quad (1)$$

This basic tool of homotopy theory not only allows to calculate homotopy groups. Different types of exact sequences also have been applied [2] in the theory of defect cores, defect transformations in phase transitions, and surface defects. Homomorphism i connects semi-defects and full defects. The elements of $\text{im } i \subset \pi_r(G/H_2)$ label those full defects, which simultaneously are semi-defects, and which are supposed to be of lowest energy. Elements of $\ker i \subset \pi_r(H_1/H_2)$ characterize semi-defects, that are unstable as full defects. The elements of $\pi_{r+1}(G/H_1)$ label defects in component 1 of the order parameter. Their dimension is reduced by one, and hence they represent boundaries. Semi-defects, which can be bounded, correspond to elements of $\text{im } \partial \subset \pi_r(H_1/H_2)$. Since the sequence is exact, and $\text{im } \partial = \ker i$, the semi-defects terminating in the bulk are exactly those, which are unstable as full defects. A semi-defect labelled by $\alpha \in \pi_r(H_1/H_2)$ can in space merge into one labelled by $\beta \in \pi_r(H_1/H_2)$, if $\partial^{-1}(\alpha\beta^{-1})$ is not empty. The elements of $\partial^{-1}(\alpha\beta^{-1}) \subset \pi_{r+1}(G/H_1)$ correspond to the possible interfacial singularities in component 1 separating the two semi-defects.

To describe semi-defects of biaxial nematic liquid crystals, we use the following groups : $G = \text{SO}(3)$, $H_1 = D_\infty$, $H_2 = D_2$. Then $\pi_2(G/H_1) = \mathbb{Z}$, $\pi_1(H_1/H_2) = \mathbb{Z}/2$, the half integers, and $\pi_1(G/H_2)$ equals $Q = \{ \pm 1, \pm i, \pm j, \pm k \}$, the group of quaternions. The exact sequence assumes the form :

$$\begin{aligned} \cdots \rightarrow \mathbb{Z} \rightarrow \mathbb{Z}/2 \rightarrow Q \rightarrow \cdots \\ s \rightarrow 2s \\ s \rightarrow i^{2s}. \end{aligned} \quad (2)$$

A point defect in the main axes of topological charge s always bounds a semi-defect of winding number $2s$. Four of the eight elements of Q correspond to semi-defects. A 2π semi-defect line can turn into a -2π line, if the interface is an $s = 1$ point singularity [8]. For the alloy of figure 2, each lattice point in the elementary cell of the superlattice corresponds to a semi-defect class. The number of semi-defect classes is always larger than or equal to that of full defects. Semi-defects are structures of their own, and not just special cases of full defects.

4. Topological classification of semi-defects : general case.

The best known examples of semi-defects are the λ lines in cholesteric liquid crystals. They are non-singular in the director field but singular in the cholesteric pitch axes [9]. If the symmetry of a representative director is $H_1 = R^3 \wedge D_\infty^x$, then the symmetry of the cholesteric phase is $H_2 = R^2 \wedge (R_h^z \wedge D_2)$. The index x in D_∞^x denotes the main rotation axis. R_h^z is the helicoidal group of axis z . There is no subgroup relation between H_1 and H_2 . To generalize the formalism of section 3, one must replace H_2 by the intersection $H_1 \cap H_2$. Then for the cholesteric liquid crystals the homotopy groups and the exact sequence become identical to those of the biaxial nematics. The λ lines, when considered as full defects, correspond to elements $i^{2s} \in Q$ [10].

Stacking faults, for example of the [111]-planes in a fcc-lattice, have not been classified by conventional topological methods [11]. With a suitable definition of the two orders they can be interpreted as semi-defects. H_2 is taken as the crystal space group. A stacking fault is generated by cutting the crystal in between two [111]-planes, moving the upper part by an element $h \in E(3)$, and gluing the two halves together again. We chose h as an operation, for which, after recombination of the crystal halves, the number of nearest neighbours of each atom is preserved. This choice is based on the phenomenological principle of the « vector equilibrium » [12]. All operations h obeying the principle form the set H_1 of « easy » motions, which in biaxial nematics corresponds to the invariance group of the main axis. As we will demonstrate in an extended article. H_1 contains all the rigid motions and the reflexions $H(P)$, that leave the uppermost plane P of the lower crystal half invariant. (Not included in $H(P)$ are « three-dimensional » symmetry elements, i.e. rotations about in-plane axes or the reflexion on P). If an element $f \in H(P)$ is not contained in the space group H_2 , then application of f to the upper crystal half moves its lowest bordering plane P' into a new position, which can also be attained *via* a translation by a fractional lattice vector $t(f)$. The operations f and $t(f)$ have the same effect on P' ($t(f)f^{-1} \in H(P')$), but in general act differently on the other planes. If we denote by T the set $\{t(f)\}$ of translations, then H_1 equals the union $H(P) \cup T$. H_1 is not a group in general, and we have to modify slightly the above used formalism. $V = G/H_2$ with $G = E(3)$ is the order parameter space of the crystal [1]. Then $A = \{kH_2 \mid k \in H_1\} \subset V$ comprises the subset of « easy positions ». Stacking faults are labelled by the elements of $\pi_0(A)$, their boundary lines by the elements of the relative homotopy group $\pi_1(V, A)$. The homotopy classes of those paths in V , which terminate on elements $t(f)H_2 \in A$ characterize partial dislocations of Burgers vector $t(f)$. The « full » crystalline line defects are related to the stacking faults and their boundaries by the exact sequence

$$\rightarrow \pi_1(V) \rightarrow \pi_1(V, A) \xrightarrow{\partial} \pi_0(A) \xrightarrow{i} \pi_0(V), \quad (3)$$

which also has been used by Mermin *et al.* [13] in the topological analysis of the cores of singularities in $^3\text{He-A}$. If G , H_1 and H_2 are all groups, we retain the sequence of the more special case (Eq. (1)).

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