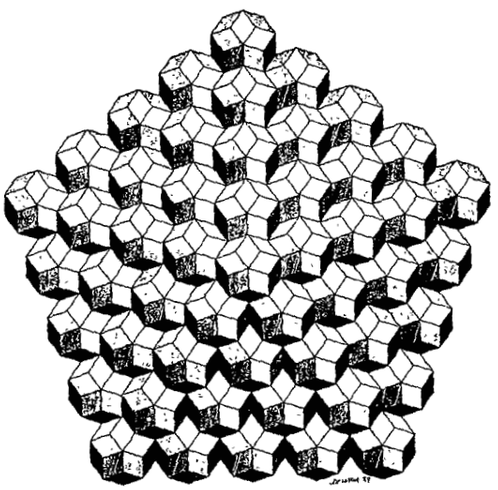
Symmetry of STRUCTURE

an interdisciplinary Symposium

Abstracts

II.



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PERFECTION AND GENEALOGY OF STRUCTURES, IN PARTICULAR, OF CRYSTAL STRUCTURES

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Whatever its nature, each structure has properties of three types: I - the properties which vary continuously and monotonically as external conditions are varied continuously and monotonically, the structure remaining unchanged; 2 - the properties which are stable in the range of external conditions permitting the existance of a given structure, but which can vary monotonically and continuously in the region of existance of a structure differing from a given structure; and 3 - the multiplicity, the properties which are fixed for any structures of a set and can in none of these structures vary continuously.

The parametric description of structures enables one to include the number F of mutually independent free parameters, the number H of differing hard parameters and also to choose a list of multiplicities M_i which form the identificator of a structure. The numbers F and H characterize any of the mutually identical elements of a structure and in combination with multiplicities M_i - perfection of a structure which means the relation between its free (F) and hard (H) origins. Changes in external conditions lead to changes in the values of free parameters up to the stabilization of some of them, accompanied by the change of the F/H ratio and, if any of M_1 is changed,

to the transition, i.e. the change of the symmetry and of the degree of perfection of a structure.

For crystal structures whose elements have a given internal symmetry (Laue class) and a given internal structure, it is possible to construct a family tree including structures with the Fedorov groups of different levels. The lowest level belongs to the Laue class of structure elements (the symmetry level is determined by the numbers F and M). The results of the parametrization are displayed in tables such as table I compiled for Laue classes (a) and Bravais lattices (b). These tables are more informative as compared with the scheme of group coordination or with the scheme of the second-kind transitions between Laue classes (Indenbom, 1960). The information needed to solve the problem about the kind of transitions is contained in the parametric descriptions of structures (Mazo, 1984): the second-kind transitions, in particular, can occur within the family tree with the participation of only one free parameter (order parameter) and it is fixed by an obligatory change of the multiplicity of identical structure elements.

There is some evidence for the adequacy of the proposed parametrization of crystal structures. The number F correlates with the number of independent components of the second-rank tensor, S (Sirotin, Shaskol'skaya, 1975). On the basis of the information about symmetry and structure of the molecule, the phase diagrams of ices and cholesteric liquid crystals were constructed. The diagrams include phases with the symmetry determined with certainty from the diffraction data, and also all

the phases whose regions of existance are determined by thermodynamic methods (Lyakhov, Mazo, 1988). The numbers H correlate with the degree of anharmonisity of structures - for the F and I type lattices the Q-factors at comparable frequencies differ; the acoustic Q-factor of alloys and compounds with the lattice cF(H=4) is lower than for alloys and compounds with the lattice cI (H=3); the Q-factor at microwave frequencies for ferrospinels (cF) is lower than for ferrogarnets (cI) and orthoferrites (oI). It is noteworthy that simple elements do not crystallize in the lattice cP(H=I), but are most frequently encountered in the cF(H=4), cI(H=3) and hP (H=2) variants.

Fig.1 (a)

F	H=0	H=1	H=2
4		$O_h(48)$-T(12)	
5	$D_{3d}(12)$-$C_3(3)$	$D_{4h}(16)$-$C_4(4)$	$D_{6h}(24)$-$C_6(6)$
6		$D_{2h}(8)$-$C_{2v}(4)$	
7		$C_{2h}(4)$-$C_2(2)$	
8			
9	$C_i(2)$-$C_1(1)$		

Fig.1 (b)

F	0	1	2	3	4
1		cP		cI	cF
2	rR	tP	hP	tI	
3		oP	oC	oI	oF
4		mP	mC		
5					
6	aP				

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