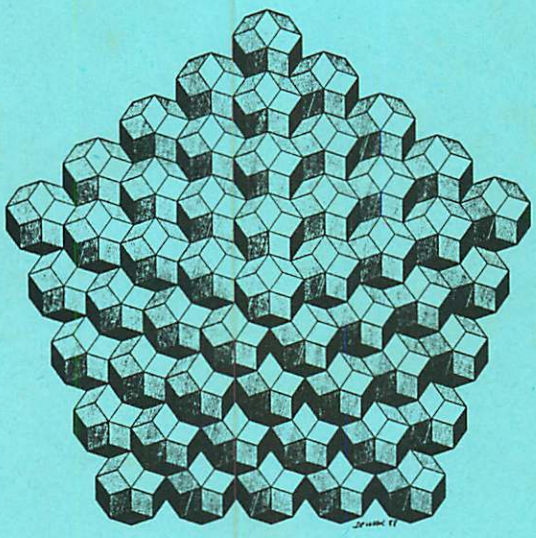
Symmetry of STRUCTURE

an interdisciplinary Symposium

Abstracts

I.



Edited by Gy. Darvas and D. Nagy

Budapest

August 13-19, 1989

hungary

SYMMETRY AS A MEASURE OF DEFECT CONTAINABILITY AND ENERGY OF CRYSTALLINE STRUCTURES

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Symmetry is characterized by the figure matchings whose number is expressed by what was qualified by E.S.Fedorov (1) a value of symmetry.

The value of symmetry (Σ) of a point class is equal to a number of faces (edges, apexes) of a general form (ν), but the same value can be deduced by multiplying a symmetry sub-group value (σ) of any face (edge, apex) by a totality of faces (edges, apexes) of a given form (2,3). The class m3m value of symmetry, for instance, is equal to 48 i.e. the maximum number of matchings as obtained through the elements of symmetry. The same value is deduced by performing the following operations:

6 cube faces (001) - 4 mm - 8.6 = 48
12 edges 110 - 2 mm - 4.12 = 48
8 apexes : 111 : - 3 m - 6.8 = 48.

Thus the value of symmetry of a point class (Σ) is a product resulting from multiplying a number of faces (edges, apexes) of general form (ν_n) by the value of symmetry proper to a facial (edge-type, apex-type) form i.e. sub-group describing the symmetry of a face, edge, apex (σ_n): $\Sigma = \nu_n \sigma_n$

The value of symmetry Σ reflects the level of energy bound within lattice. Values of Σ do not change monotonously and can be conformable with the well known set of whole rational numbers: 1,2,3,4,6, 8,12,16,24,48. It is easily understood that Σ is a discrete function having the aspect (Fig.1):

$$f(K) \begin{cases} 1,, \text{ if } K=1 \\ 2^{k/2}, \text{ if k is an even number} \\ 3.2\,\frac{k-2}{2}, \text{ if k is an odd number.} \end{cases}$$

Mechanical, radiation, heat and other effects generate defects in the crystal structure thus disturbing the lattice site order. The critical number of defects that the structure may contain before it becomes amorphous is limited by a defect saturation level

(Dk). The level of defect containability saturation characterizes free (excess) crystal energy.

Thus the cumulative lattice energy is made up with intrinsic (bound) energy proportional to the value of symmetry and therefore changing discretely, on the one side, and free (excess) energy which grows and relaxes monotonously, on the other side. From this it transpires that the properties of ideal (defectless) crystals change in compliance with "quantum numbers" of symmetry, while for actual crystals quantation is shaded by energies of a huge number of structural defects.

Quantized physical properties are also characteristic to polymorphous transformations accompanied by jumps of symmetry values. As this takes place, Σ values may drop from high to low bypassing intermediate numbers (diamond, graphite) or else they follow a sequence of quantation degrees (cristobalite - tridymite - quartz).

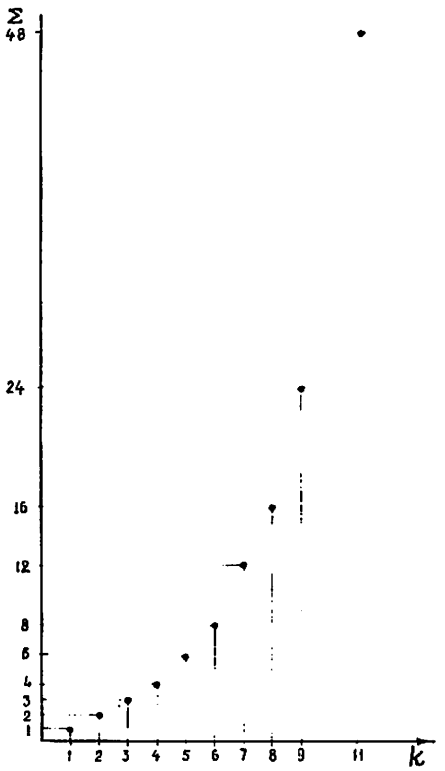
As for the ideal crystals, their quantized properties appear either at very low temperatures or with very fine individuals, such as fine metal particles, whiskers, particle fragments.

Polyform quartz species provide a classical example of how the physical properties are quantized depending on a descrete application of Σ values.

At high temperatures in isotropic medium (under a normal pressure) forms β-cristobalite featuring the value of symmetry $\Sigma = 48$. This is a manifestation P.Curie principle of symmetry superposition, namely, a highly symmetrical (and highly energetical) medium generates a highly symmetrical and highly energetical structure. Under the action of external factors (mechanical, radiational) the β-cristobalite becomes defect saturated to form α- cristobalite with $\Sigma = 16$. Intrinsic lattice energy lowers, while the defect containability level grows. Under the further-on external impact the structures being formed are progressively lower symmetrical until they reach $\Sigma = 4$ (coesite), the silica properties alter in a discrete manner, too - lattice parameters, refraction characteristics, spectral features (see the Table).

Twins are characteristic to the structure of quartz and its polyformous modifications. The readiness to twin formation should be considered as a manifested lattice energy quantation localized within a structural volume. The twin symmetry boundary is above (or beneath) that of monocrystals. Therefore "breaking" of a crystal into twin sub-individuals means a texturized distribution of bound energy U and free energy D.

Fig.1 Discrete function $\Sigma(K)$



SiO_2 properties quantizing as a function of value of Symmetry Σ

Polymorphous modification	Chemical formula	Molecular mass	Value of symmetry Σ	Parameters of elementary sell a_o	b_o	c_o	Volume of elementary sell, A^3	Specific mass	Refraction parameters N_g	N_p	X cm^{-1}
I	2	3	4	5	6	7	8	9	I0	II	I2
β-cristobalite	β-SiO_2	60.084	48	7.II	-	-	360.94	2.I9	I.487	-	II98 I096 793.7
α-cristobalite	α-SiO_2	60.084	8	4.97	-	6.93	I7I.I8	2.32	I.486	I.484	-
β-tridymite	β-SiO_2	60.084	24	5.04	-	8.24	I8I.26	2.I8	I.474	I.469	II05 787 568
α-tridymite	α-SiO_2	60.084	8	9.90	I7.I	I6.3	22I3.84	2.3I	I.483	I.479	-
β-quartz	β-SiO_2	60.084	I2	4.999	-	5.457	II8.I0	2.53	I.539	I.53I	-
α-quartz	α-SiO_2	60.084	6	4.9I3	-	5.405	II2.07	65.	I.565	I.544	II59 I093 693
Stishovite	SiO_2	60.084	I6	4.I79	-	2.665	46.54	4.33	I.826	I.799	9.49 769 672 885 730 623
Kitite	SiO_2	60.084	8	7.456	-	8.604	478.3I	2.50	I.522	I.5I3	-
Coesite	SiO_2	60.084	4	7.23	I2.52 β =I20°	7.23	566.76	3.03	I.597	I.594	I2I8 II52 I07

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