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CHANGES OF ELASTIC CONSTANTS IN STRUCTURAL PHASE TRANSITIONS. I. NON-ELASTIC PHASE TRANSITIONS*

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The tensor of the elastic constants in the vicinity of the structural phase transition is considered in the framework of the phenomenological theory. The behaviour and changes of the elastic constants associated with all equi-translational non-elastic structural phase transitions induced by a one-dimensional irreducible representation of the high symmetry group, are found on the basis of the symmetry relations. With the aid of the renormalization group approach, it is established which elastic constants show a critical behaviour.

1. *Introduction*

The behaviour of the elastic constants of a crystal in the vicinity of the structural phase transition point can be considered in the framework of the phenomenological theory of Landau and Lifshitz [1, 2]. The main idea of a reduction of the symmetry of a crystal by an active mode which is associated with the relevant irreducible representation involves specific changes of the elastic constants. These changes depend upon the symmetry of the high and low symmetry phase and on the active irreducible representation.

Phase transitions can be divided into non-elastic and elastic ones. The non-elastic phase transition is associated with an active mode whose symmetry differs from that of any of the normal homogeneous strains of the crystal. Hence it follows that the equi-translational phase transitions with an active mode in the center of the Brillouin zone which has not the symmetry of the normal strain, and all phase transitions accompanied by an enlargement of the unit cell with the wave vector out of the center of the Brillouin zone, are non-elastic. In the elastic phase transition the symmetries of the active normal mode and of one of the normal strains are the same. The phase transition from hexagonal β-quartz ($P6_222$) (point group 622) to trigonal α-quartz ($P3_121$) (point group 32) at 846K induced by B_2 irreducible representation at $\boldsymbol{k} = 0$ is an example of the non-elastic phase transition [3].

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Taking into account the symmetry of the phase and the symmetry of the active normal mode, it is possible, on the basis of the phenomenological theory, to describe the temperature behaviour of the elastic constants in the vicinity of the phase transition point [4]. However, the critical fluctuations of the active normal mode are, as a rule, coupled to the elastic degree of freedom. For non-elastic phase transitions associated with one-dimensional irreducible representation the result is as follows. The elastic constants which describe the totally symmetric strain which in fact denotes the dilatation of the crystal show temperature behaviour different from predictions of the phenomenological theory. Moreover, such critical behaviour of the elastic constant is expected to lead to the first order phase transition, except when the critical temperature does not change under hydrostatic pressure. Then the phase transition associated with a one-dimensional irreducible representation remains of the second order.

We start off with the free energy expansion in terms of the active normal mode amplitudes and the normal strains and next derive the set of equilibrium equations, and the formula which describes the behaviour of the elastic constants in a vicinity of the phase transition. The elastic constants are written explicitly for equi-translational non-elastic phase transitions with the active normal mode which transforms according to a one-dimensional irreducible representation. To decide whether a given elastic constant is modulated by the critical fluctuations we set up the local free energy density in the hydrodynamic limit and derive a set of the renormalization group recurrence relations. The elastic phase transitions will be discussed in the next paper [5].

2. *The phenomenological theory*

A state of a crystal can be described by temperature T and the components of the symmetric strain tensor V_i^0 ($i = 1, 2 \dots 6$ — the usual Voigh notation). Components V_i^0 specify a homogeneous strain of the crystal. Under a set of symmetry elements which form a space group of a crystal its density is invariant. The irreducible representations of the space group, in turn, are indexed by the wave vector $\boldsymbol{k}$ and the number of the irreducible representation of the little group. The homogeneous strain of an infinite wavelength, is classified by $\boldsymbol{k} = 0$ and irreducible representations of the point group of the crystal.

It is convenient to introduce the normal strain components S_α^0, $\alpha = 1, 2, \dots 6$, so that

$$S_\alpha^0 = \sum_i \sigma_i(\alpha) V_i^0. \tag{1}$$

Coefficients $\sigma_i(\alpha)$ are the eigenvectors of the bare elastic constant tensor c_{il}, namely

$$\sum_l c_{il}\sigma_l(\alpha) = c_\alpha \sigma_i(\alpha). \tag{2}$$

The $\sigma_i(\alpha)$ are real and orthonormal [6]. The six-component eigenvector $\sigma(\alpha)$ transforms according to one of the irreducible representation Γ_α of the point group of the crystal. S_α^0 denotes the amplitude of a given normal strain. For example, the general strain in a cubic crystal with the point group $m3m$ can be decoupled into $A_{1g}+E_g+T_{2g}$ irreducible representations, and then the corresponding normal elastic constants are $c_{11}+2c_{12}$, $c_{11}-c_{12}$ and c_{44}.

The free energy of a crystal $F = F(T, S_1^0, S_2^0, \ldots S_6^0, \{Q_{kj}^0\})$ is a function of temperature T and the homogeneous strain S_α^0. It is useful, however, to introduce, apart from independent variables T and S_α^0, a set of dependent variables, i.e. a set of the generalized normal modes amplitudes Q_{kj}^0. Each normal mode is specified by an irreducible representation of the space group Γ_{kj} i.e. by a particular wave vector $\boldsymbol{k}$ and the irreducible representation of the relevant little group. Index j numbers both the irreducible representation of the little group and its components. The normal mode amplitude may concern a wave of an additional displacement either of atoms or a group of atoms to the homogeneous strain of the Bravais lattice. In molecular crystals Q_{kj}^0 may describe a wave of twist of molecular groups. The normal amplitude Q_{kj}^0 may also denote the wave of probability of occupation of one of the equivalent states in a crystal in which the number of sites in the lattice for atoms of a given kind is in excess over the number of atoms. This also concerns the case of different static orientations occurring in molecular crystals.

The normal mode amplitudes Q_{kj}^0 are not independent variables. They are adjusted in such a way that at a given value of external conditions i.e. temperature T and strain S_α^0 the free energy $F = F(T, S_1^0, S_2^0, \ldots S_6^0, \{Q_{kj}^0\})$ achieves a minimum for a correct value of Q_{kj}^0. Thus, the Q_{kj}^0' s are the solutions of the following set of equations for the extremum of the free energy

$$\left.\frac{\partial F}{\partial Q_{kj}^0}\right|_0 = 0, \tag{3}$$

which allows one to express Q_{kj}^0 as a function of the normal strain S_α^0. The derivatives are taken at the equilibrium configuration. Knowing the amplitudes of the normal strains one finds the normal stresses

$$p_\alpha = \left.\frac{\partial F}{\partial S_\alpha}\right|_0 \tag{4}$$

which keep the crystal in the deformed state.

Consider the phase transition from high to low symmetry phase accompanied by the symmetry reduction from the space group G_s to the space F_s, F_s being a subgroup of G_s. For the high symmetry phase let us choose all the normal strains and normal modes amplitudes to be zero. Then, the free energy expanded around the point $S_\alpha^0 = 0$ and $Q_{kj}^0 = 0$ can be written in the form

$$\begin{aligned} F = F(T, \{0\}, \{0\}) + \tfrac{1}{2}\sum_{\alpha} c_\alpha (S_\alpha^0)^2 + \sum_{\alpha}\sum_{kj} U_\alpha(\boldsymbol{k}, j) S_\alpha^0 Q_{kj}^0 \\ + \tfrac{1}{2}\sum_{kj} \lambda_{kj} Q_{kj}^0 Q_{-kj}^0 + \tfrac{1}{2}\sum_{\alpha\beta}\sum_{kj} K_{\alpha\beta}(\boldsymbol{k}, j) S_\alpha^0 S_\beta^0 Q_{kj}^0 \\ + \tfrac{1}{2}\sum_{\alpha}\sum_{kjj'} L_\alpha(\boldsymbol{k}, j, j') S_\alpha^0 Q_{kj}^0 Q_{-kj'} + \tfrac{1}{6}\sum_{\alpha\beta\gamma} c_{\alpha\beta\gamma} S_\alpha^0 S_\beta^0 S_\gamma^0 \\ + \tfrac{1}{24}\sum_{\substack{k_1k_2k_3k_4\\ j_1j_2j_3j_4}} B\begin{pmatrix} \boldsymbol{k}_1 & \boldsymbol{k}_2 & \boldsymbol{k}_3 & \boldsymbol{k}_4 \\ j_1 & j_2 & j_3 & j_4 \end{pmatrix} Q_{k_1j_1}^0 Q_{k_2j_2}^0 Q_{k_3j_3}^0 Q_{k_4j_4}^0 \delta(\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3+\boldsymbol{k}_4). \end{aligned} \tag{5}$$

Depending on the physical meaning of the normal mode amplitude the diagonal coefficient of the harmonic term λ_{kj} may represent either the square of the energy of a phonon from branch j and for the wave vector $\boldsymbol{k}$, or an excess of the free energy produced by the probability occupation wave. The third order term of the normal mode amplitude has been omitted because it vanishes for one-dimensional irreducible representation. Nevertheless, this term may exist for some multidimensional representation, but then it leads to the first order phase transition.

Each term of the free energy expansion formula should be invariant under the symmetry elements of the crystal point group of the high symmetry phase. In consequence the expression of direct products of the irreducible representation of a normal strain Γ_α and normal mode Γ_{kj} created according to the form of a given term of the free energy expansion has to contain the totally symmetric irreducible representation, otherwise it vanishes. In particular, the linear coupling term between the normal strain and normal mode vanishes provided Γ_{kj} is described by the non-zero wave vector $\boldsymbol{k}$, since then the direct product $\Gamma_\alpha \otimes \Gamma_{kj}$ does not contain the totally symmetric irreducible representation. Similar discussion for the $K_{\alpha\beta}(\boldsymbol{k}, j)$ term leads us to the common conclusion that

$$U_\alpha(\boldsymbol{k}, j) = \delta_{\boldsymbol{k},0} U_\alpha(\boldsymbol{k}, j), \qquad K_{\alpha\beta}(\boldsymbol{k}, j) = \delta_{\boldsymbol{k},0} K_{\alpha\beta}(j). \tag{6}$$

This is a consequence of the translational invariance of a crystal lattice. So, in the case of phase transitions accompanied by an enlargement of a unit cell terms $U_\alpha(\boldsymbol{k}, j)$ and $K_{\alpha\beta}(\boldsymbol{k}, j)$ are insignificant, and the phase transition cannot be of elastic type. Notice, however, that some components of $L\,(\boldsymbol{k}, j, j')$ coefficients may always be present, namely those for which Γ_α transforms according to the totally symmetric irreducible representation.

The reduction of symmetry in the high symmetry phase is produced by the active normal modes which transform according to one irreducible representation of the space group G_s, therefore, the summation over $\boldsymbol{k}$ and j in (5) can be confined to $\boldsymbol{k}_c$ — the arms of the critical star and to j_c — the components of the irreducible representation of the relevant little group. For multidimensional representations further restrictions on the summation over $\boldsymbol{k}_c$ and j_c can be imposed [7].

The normal strains and normal amplitudes which occur in expansion (5) may be treated as either fluctuations in the high symmetry phase or a sum of a new equilibrium state of a low symmetry phase described by S_α and Q_{kj}, and fluctuations s_α and q_{kj} around that equilibrium state S_α and Q_{kj}. Accepting the last, we insert into (5) $S_\alpha^0 = S_\alpha + s_\alpha$ and $Q_{kj}^0 = Q_{kj} + q_{kj}$ and rearrange the expansion of the free energy with the aid of the familiar procedure of completing the square. In result, one finds

$$F = F(T, \{S_\alpha\}, \{Q_{k_c j_c}\}) + \sum_\alpha p_\alpha s_\alpha + \tfrac{1}{2} \sum_{\alpha\beta} \Big[c_\alpha \delta_{\alpha,\beta} + \sum_\gamma c_{\alpha\beta\gamma} S_\gamma$$

$$+ \sum_{j_c} \delta_{k_c,0} K_{\alpha\beta}(j_c) Q_{k_c j_c} - \sum_{k_c j_c} \sum_{k_c' j_c'} N_\alpha(k_c, j_c) M \begin{pmatrix} k_c & k_c' \\ j_c & j_c' \end{pmatrix} N_\beta(k_c', j_c') \Big] s_\alpha s_\beta$$

$$+\tfrac{1}{2}\sum_{k_c j_c}\sum_{k_c' j_c'} R\begin{pmatrix} k_c & k_c' \\ j_c & j_c' \end{pmatrix} t_{k_c j_c} t_{k_c' j_c'} + \tfrac{1}{6}\sum_{\alpha\beta\gamma} c_{\alpha\beta\gamma} s_\alpha s_\beta s_\gamma$$

$$+\tfrac{1}{2}\sum_{\alpha\beta}\sum_{j_c} \delta_{k_c,0} K_{\alpha\beta}(j_c) s_\alpha s_\beta q_{k_c j_c} + \tfrac{1}{2}\sum_{\alpha}\sum_{k_c j_c j_c'} L_\alpha(k_c, j_c, j_c') s_\alpha q_{k_c j_c} q_{-k_c j_c'} + \dots, \tag{7}$$

where

$$N_\alpha(k, j) = \delta_{k,0} U_\alpha(j) + \delta_{k,0} \sum_\beta K_{\alpha\beta}(j) S_\beta + \sum_{j'} L_\alpha(k, j, j') Q_{kj'} \tag{8}$$

$$R\begin{pmatrix} k & k' \\ j & j' \end{pmatrix} = [\lambda_{kj}\delta_{j,j'} + \sum_\alpha L_\alpha(k, j, j') S_\alpha]\delta(k+k')$$

$$+\tfrac{1}{2}\sum_{\substack{k_1 k_2 \\ j_1 j_2}} B\begin{pmatrix} k & k' & k_1 & k_2 \\ j & j' & j_1 & j_2 \end{pmatrix} Q_{k_1 j_1} Q_{k_2 j_2} \delta(k+k'+k_1+k_2) \tag{9}$$

and

$$t_{kj} = q_{kj} + \sum_\alpha \sum_{kj} M\begin{pmatrix} k & k' \\ j & j' \end{pmatrix} N_\alpha(k', j') s_\alpha, \tag{10}$$

and

$$\sum_{k'j'} M\begin{pmatrix} k & k' \\ j & j' \end{pmatrix} R\begin{pmatrix} k' & k'' \\ j' & j'' \end{pmatrix} = \delta_{k,k''}\delta_{j,j''}. \tag{11}$$

The zeroth term $F(T, S_1, S_2, \dots S_6, \{Q_{k_c j_c}\})$ corresponds to the free energy of the new low symmetry phase, p_α is the stress component acting on the new phase. Some insignificant terms have been neglected.

The equilibrium values of the normal deformation S_α and the active normal mode $Q_{k_c j_c}$ which arise in the low symmetry phase as a result of the symmetry reduction can be found from equilibrium equations (3) and (4) which now take the form

$$p_\alpha + c_\alpha S_\alpha + \sum_{j_c} \delta_{k_c,0} U_\alpha(j_c) Q_{k_c j_c} + \sum_\beta \sum_{k_c j_c} \delta_{k_c,0} K_{\alpha\beta}(j_c) Q_{k_c j_c} S_\beta + \tfrac{1}{2}\sum_{\beta\gamma} c_{\alpha\beta\gamma} S_\beta S_\gamma$$

$$+\tfrac{1}{2}\sum_{k_c j_c j_c'} L_\alpha(k_c, j_c, j_c') Q_{k_c j_c} Q_{-k_c j_c'} = 0 \quad \text{for} \quad \alpha = 1, 2, \dots 6, \tag{12}$$

$$\sum_\alpha U_\alpha(k_c, j_c) S_\alpha + \tfrac{1}{2}\sum_{\alpha\beta} \delta_{k_c,0} K_{\alpha\beta}(j_c) S_\alpha S_\beta + \sum_{k_c' j_c'} \Bigg\{ \tfrac{2}{3}\Bigg[\lambda_{k_c j_c}\delta_{j_c, j_c'}$$

$$+ \sum_\alpha L_\alpha(k_c, j_c, j_c') S_\alpha \Bigg] \delta(k_c + k_c') + \tfrac{1}{3} R\begin{pmatrix} k_c & k_c' \\ j_c & j_c' \end{pmatrix} \Bigg\} Q_{k_c' j_c'} = 0. \tag{13}$$

To find the effective elastic constants c_{il} in the Voigh notation one takes the second derivative of the free energy with respect to the normal strain and with the help of the eigenvectors $\sigma_i(\alpha)$ (1) transforms it into the form

$$\tilde{c}_{il} = \sum_{\alpha\beta} \sigma_i(\alpha)\tilde{c}_{\alpha\beta}\sigma_l(\beta); \quad \tilde{c}_{\alpha\beta} = \frac{\partial^2 F}{\partial s_\alpha \partial s_\beta}. \tag{14}$$

From (7), one finds

$$\tilde{c}_{il} = c_{il} + \sum_{j_c} \delta_{\boldsymbol{k}_c,0} K_{il}(j_c) Q_{\boldsymbol{k}_c j_c} + \sum_n c_{iln} V_n$$

$$-\sum_{\boldsymbol{k}_c j_c} \sum_{\boldsymbol{k}_c' j_c'} N_i(\boldsymbol{k}_c, j_c) M \begin{pmatrix} \boldsymbol{k}_c & \boldsymbol{k}_c' \\ j_c & j_c' \end{pmatrix} N_l(\boldsymbol{k}_c', j_c'), \tag{15}$$

where

$$N_i(\boldsymbol{k}_c, j_c) = \sum_\alpha \sigma_i(\alpha) N_\alpha(\boldsymbol{k}_c, j_c), \tag{16}$$

and

$$V_n = \sum_\alpha \sigma_n(\alpha) S_\alpha \tag{17}$$

are those components of the strain tensor which result from the symmetry reduction at the phase transition point. The strains and the normal mode amplitudes appearing in (15) should be found from the equilibrium equations (12) and (13).

3. Equi-translational non-elastic phase transitions

Consider the equi-translational phase transition induced by one-dimensional irreducible representation $\Gamma_{0 j_c}$. Let the normal strain be represented by the irreducible representation Γ_α. The star of $\boldsymbol{k}_c = 0$ consists of one wave vector only. Let us establish the vanishing components of $U_\alpha(j_c)$, $L_\alpha(0, j_c, j_c)$, and $K_{\alpha\beta}(j_c)$. (*i*) If $\Gamma_{0 j_c}$ and Γ_α are not the same, component $U_\alpha(j_c) = 0$. (*ii*) If Γ_α is not the totally symmetric representation, component $L_\alpha(0, j_c, j_c) = 0$. (*iii*) If the direct product $\Gamma_\alpha \otimes \Gamma_\beta$ does not include $\Gamma_{0 j_c}$, $K_{\alpha\beta}(j_c) = 0$. In particular, if Γ_α is the totally symmetric irreducible representation, components $K_{\alpha\alpha}(j_c) = 0$. (*iv*) Also, if Γ_α is a totally symmetric irreducible representation and $\Gamma_{0 j_c}$ is not the same as any of Γ_α, $\sum_\beta K_{\alpha\beta}(j_c) S_\beta = 0$.

The phase transition can be called non-elastic if all the components $U_\alpha(j_c)$ ($\alpha = 1, 2, \ldots, 6$) vanish. Then, equilibrium equations (12) decouple into two subsystems. Owing to statement (*iv*) for the Γ_α which correspond to the totally symmetric representation, we have

$$c_\alpha S_\alpha + \tfrac{1}{2} L_\alpha(0, j_c, j_c) Q_{0 j_c}^2 = 0, \tag{18}$$

and for Γ_α not being the totally symmetric representation

$$c_\alpha S_\alpha + Q_{0 j_c} \sum_\beta K_{\alpha\beta}(j_c) S_\beta = 0. \tag{19}$$

We have assumed $p_\alpha = 0$ and neglected the square term in strain. From (19) and from statement (*iii*), we conclude that in the low symmetry phase the static deformation components S_α, which transform according to any other than totally symmetric representation, remain zero. Hence

$$\sum_{\alpha\beta} K_{\alpha\beta}(j_c) S_\alpha S_\beta = 0, \tag{20}$$

the remaining equilibrium equation (13) is then

$$\left\{\lambda_{0j_c} + \sum_\alpha L_\alpha(0, j_c, j_c) S_\alpha + \tfrac{1}{6} B\begin{pmatrix}0\\ j_c\end{pmatrix} Q_{0j_c}^2\right\} Q_{0j_c} = 0. \tag{21}$$

As usual, we assume the expansion coefficients to be temperature independent except for $\lambda_{0j_c}(T)$ which is a linear function of temperature. The critical temperature T_c for the normal mode subsystem is defined by $\lambda_{0j_c}(T_c) = 0$. The amplitude of the normal active mode Q_{0j_c} and totally symmetric normal strain S_α can be obtained as a solution of equations (18) and (21). Then, in the region where $\lambda_{0j_c} > 0$, say above T_c, we have $Q_{0j_c} = S_\alpha = 0$ and

$$R(0, j_c, T) = \lambda_{0j_c}(T) > 0, \tag{22}$$

where $R(0, j_c, T)$ stands for the temperature dependence of $R\begin{pmatrix}0 & 0\\ j_c & j_c\end{pmatrix}$ (9). In the region below T_c, where $\lambda_{0j_c}(T) < 0$, we have

$$Q_{0j_c} = \pm \left\{6\lambda_{0j_c}(T)\left[B\begin{pmatrix}0\\ j_c\end{pmatrix} - 3\sum_\alpha c_\alpha^{-1} L_\alpha(0, j_c, j_c)\right]^{-1}\right\}^{1/2} \sim |T-T_c|^{1/2},$$

and

$$S_\alpha = -\tfrac{1}{2} c_\alpha^{-1} L_\alpha(0, j_c, j_c) Q_{0j_c}^2 \sim |T-T_c|,$$

and

$$R(0, j_c, T) = -2\left[\lambda_{0j_c}(T) + \sum_\alpha L_\alpha(0, j_c, j_c) S_\alpha(T)\right] > 0. \tag{23}$$

One also finds that $\sum_\alpha L_\alpha(0, j_c, j_c) S_\alpha$ is always negative. The function $R(0, j_c, T)$ is equal to zero at T_c and remains positive above and below the critical point. It is at least twice steeper below than above the critical point.

Basing on formula (15) the effective elastic constants can easily be calculated in the following manner. First the symmetry tensor $L_i(0, j_c, j_c)$ and $K_{il}(j_c)$ have to be found for a given active irreducible representation Γ_{0j_c}. To do this we expand point group G of the high symmetry phase over subgroup F being the point group of the low symmetry phase i.e. $G = \sum_h g_h F$, where g_h is a generating symmetry element in which g_1 is the identity operation. The active irreducible representation Γ_{0j_c} becomes the totally symmetric representation in F and consequently its characters in F are all $+1$. The symmetric tensor of second

TABLE I

Tensors of elastic constants in a vicinity of equi-translational non-elastic phase transitions induced by one-dimensional irreducible representations

	c_{il}						G	Γ_{0j_c}	F
Monoclinic	A	F	D	0	I	0	$2/m$ $(2\|\|Y)$	A_u	2
		E	G	0	J	0		B_u	m
			C	0	M	0			
				c_{44}	0	c_{46}			
					H	0			
						c_{66}			
Orthorhombic	A	F	D	0	0	0	mmm	A_u	222
		E	G	0	0	0		B_{1u}	$mm2$
			C	0	0	0		B_{2u}	$mm2$
				c_{44}	0	0		B_{3u}	$mm2$
					c_{55}	0			
						c_{66}			
Tetragonal	A	B	D	0	0	c_{16}	$4/m$	A_u	4
		A	D	0	0	$-c_{16}$		B_u	$\bar{4}$
			C	0	0	0			
				c_{44}	0	0			
					c_{44}	0			
						c_{66}			
	A	B	D	0	0	i	$4/mmm$	A_{2g}	$4m$
		A	D	0	0	$-i$	$\bar{4}2m$	A_2	$\bar{4}$
			C	0	0	0	422	A_2	4
				c_{44}	0	0	$4mm$	A_2	4
					c_{44}	0			
						c_{66}			
	A	B	D	0	0	0	$4/mmm$	A_{1u}	422
		A	D	0	0	0		A_{2u}	$4mm$
			C	0	0	0		B_{1u}	$\bar{4}2m$
				c_{44}	0	0		B_{2u}	$\bar{4}2m$
					c_{44}	0			
						c_{66}			
Trigonal	A	B	D	c_{14}	$-c_{25}$	0	$\bar{3}$	A_u	3
		A	D	$-c_{14}$	c_{25}	0			
			C	0	0	0			
				c_{44}	0	c_{25}			
					c_{44}	c_{14}			
						c_{66}			
	A	B	D	l	0	0	$\bar{3}m$	A_{2g}	$\bar{3}$
		A	D	$-l$	0	0	$3m$	A_2	3
			C	0	0	0	32	A_2	3

TABLE I (continued)

	C_{il}						G	Γ_{0j_c}	F
Trigonal				c_{44}	0	0			
					c_{44}	l			
						c_{66}			
	A	B	D	c_{14}	0	0	$\bar{3}m$	A_{1u}	32
		A	D	$-c_{14}$	0	0		A_{2u}	$3m$
			C	0	0	0			
				c_{44}	0	0			
					c_{44}	c_{14}			
						c_{66}			
Hexagonal	A	B	D	l	$-j$	0	$6/m$	B_g	3
		A	D	$-l$	j	0	$\bar{6}$	A''	3
			C	0	0	0	6	B	3
				c_{44}	0	j			
					c_{44}	l			
						c_{66}			
	A	B	D	0	$-j$	0	$6/mmm$	B_{1g}	$\bar{3}m$
		A	D	0	j	0	$\bar{6}m2$	A_1''	32
			C	0	0	0	$6mm$	B_1	$3m$
				c_{44}	0	j	622	B_1	32
					c_{44}	0			
						c_{66}			
	A	B	D	l	0	0	$6/mmm$	B_{2g}	$\bar{3}m$
		A	D	$-l$	0	0	$\bar{6}m2$	A_2''	$3m$
			C	0	0	0	$6mm$	B_2	$3m$
				c_{44}	0	0	622	B_2	32
					c_{44}	l			
						c_{66}			
	A	B	D	0	0	0	$6/mmm$	A_{1u}	622
		A	D	0	0	0		A_{2g}	$6/m$
			C	0	0	0		A_{2u}	$6mm$
				c_{44}	0	0		B_{1u}	$\bar{6}2m$
					c_{44}	0		B_{2u}	$\bar{6}2m$
						c_{66}	$\bar{6}2m$	A_2'	$\bar{6}$
							$6mm$	A_2	6
							622	A_2	6
							$6/m$	A_u	6
								B_u	6
Cubic	A	B	B	0	0	0	$m3m$	A_{1u}	432
		A	B	0	0	0		A_{2g}	$m3$
			A	0	0	0		A_{2u}	$\bar{4}3m$
				c_{44}	0	0	432	A_2	23
					c_{44}	0	$\bar{4}3m$	A_2	23
						c_{44}	$m3$	A_2	23

$L^{(F)}(0, j_c, j_c)$ and fourth $K^{(F)}(j_c)$ rangs for the subgroup F (and totally symmetric representation in F) are tabulated in [4] in Voigh notation. Their symmetries which arise under the operation g_h can be ound by means of the usual transformation matrices $P_L(g_h)$ and $P_K(g_h)$. Now, according to the form of the terms $L_i(0, j_c, j_c)\ V_i Q^2_{0j_c}$ and $K_{il}(j_c) V_i V_l Q_{0j_c}$ in (5) the symmetries of these tensors come out as a result of averaging over the cosets $g_h F$ with an apropriate factor made up from character $\chi_{0j_c}(g_h)$ of the representation Γ_{0j_c} in G. Thus

$$L(0, j_c, j_c) = \sum_h \chi^2_{0j_c}(g_h) P_L(g_h) L^{(F)}(0, j_c, j_c),$$

$$K(0, j_c, j_c) = \sum_h \chi_{0j_c}(g_h) P^T_K(g_h) K^{(F)}(j_c) P_K(g_h). \tag{24}$$

Taking advantages of (15), (16) and (8) we find the effective elastic constants in vicinity of all equi-translational non-elastic phase transitions induced by one-dimensional irreducible representations. In Table I are quoted the tensors of the elastic constants, the point group G of the high symmetry phase, the associated irreducible representation of the active normal mode of the high symmetry group, and the point group F of the low symmetry phase [6]. Abbreviations are listed in Table II. The tensors of the elastic constants are written in conventional coordinate systems with respect to the high symmetry phase. They also

TABLE II

Summary of abbreviations

$R = R(0, j_c, T)$	$L_i = L_i(0, j_c, j_c)$
$Q = Q_{0j_c}$	$K_{il} = K_{il}(j_c)$
$A = c_{11} - L^2_1 Q^2 R^{-1}$	$H = c_{55} - L^2_5 Q^2 R^{-1}$
$B = c_{12} - L^2_1 Q^2 R^{-1}$	$I = c_{15} - L_1 L_5 Q^2 R^{-1}$
$C = c_{33} - L^2_3 Q^2 R^{-1}$	$J = c_{25} - L_2 L_5 Q^2 R^{-1}$
$D = c_{13} - L_1 L_3 R^{-1}$	$M = c_{35} - L_3 L_5 Q^2 R^{-1}$
$E = c_{22} - L^2_2 Q^2 R^{-1}$	$i = K_{16} Q$
$F = c_{12} - L_1 L_2 Q^2 R^{-1}$	$j = K_{15} Q$
$G = c_{23} - L_2 L_3 Q^2 R^{1}$	$l = K_{14} Q$

agree with the conventional coordinate systems of the arising low symmetry phase, one exception being the tensor of low symmetry phase with a point group $\bar{3}m$, $3m$, $3m$, 32 which arise from $6/mmm$, $\bar{6}m2$, $6mm$, 622 by B_{2g}, A_2'', B_2 and B_2 irreducible representation, respectively, and is turned around axis z by 30° with respect to the triclinic conventional system. The elements of the tensor written in the conventional form c_{44}, c_{14} and so on, do not vary across the phase transition point provided the phase transition is of second order. Also the difference c_{11}–c_{12} remains constant in all non-elastic phase transitions, the exception being the phase transitions from $2/m$ to either 2 or m point groups. The temperature dependence of the elastic constants in the frame of the phenomenological theory can be estimated with the assumption that only $Q_{0j_c}(T)$ and $R(0, j_c, T)$ are temperature dependent. In result the elastic constants of type i, j, and l are proportional to the temperature dependence of the order parameter. The elastic constants of type from A to M may exhibit a discontinuity at T_c, since $Q^2_{0j_c}$ and $R(0, j_c, T)$ have the same temperature dependence below T_c. Such elastic constants are related to the totally symmetric strain or, in other words, to dilatation of the crystal and, as it will be shown below, they are sensitive to the critical fluctuations of the active normal mode. In consequence, they show a remarkable critical behaviour in vicinity of T_c. This effect may lead to the first order phase transition. The elastic constants listed in Table I are not corrected for the discontinuous volume change associated with the first order phase transition.

The special properties of the elastic constants of the type from A to M are due to the coupling constant $L_\alpha(0, j_c, j_c)$ between the square of the normal mode amplitude and the elastic strain. In a special case, however, when the critical temperature does not change under the deformation of the crystal i.e. $dT_c/dV_i = 0$, we have $L_i(0, j_c, j_c) = 0$. This is established as follows. Suppose the crystal in the high symmetry phase, where $Q_{0j_c} = 0$, is deformed by an amount δS_α. In the deformed state critical temperature T_d is defined by $R\begin{pmatrix} 0 & 0 & T_d \\ j_c & j_c & \end{pmatrix} = 0$. Expanding $\lambda_{0j_c}(T)$ around T_c, we get the critical temperature for the deformed state

$$T_d = T_c - \left(\frac{d\lambda_{0jc}}{dT}\right)^{-1} \sum_\alpha L_\alpha(0, j_c, j_c)\delta S_\alpha, \tag{25}$$

where α runs over the totally symmetric irreducible representations only. Since $d\lambda_{0j_c}/dT \neq 0$ (usual positive), we find $T_d = T_c$ if $L_\alpha(0, j_c, j_c) = 0$. Concluding, the critical temperature does not change under homogeneous strain if the coefficients $L_\alpha(0, j_c, j_c)$ are equal zero. In this special case, a dilatation caused by a hydrostatic pressure does not influence the critical temperature. It is, however, essential to note that normal strain δS_α of a shear strain type has always little influence on the value of T_d, since the $L_\alpha(0, j_c, j_c)$ for Γ_α which is not the totally symmetric irreducible representation, vanishes by symmetry.

If the high symmetry phase is a one domain phase, the low symmetry phase consists of two types of domains characterized by $+Q_{0j_c}$ and $-Q_{0j_c}$. Therefore, these elastic constants which are proportional to Q_{0j_c}, will be different in those domains.

4. *Renormalization group approach*

The phenomenological theory does not take into account the critical fluctuations. Some elastic constants show, however, a critical behaviour close to the phase transition point, others are not sensitive to that. To study these relations we derive the renormalization group equations for all relevant coupling constants. It will be assumed that the intrinsic critical behaviour occurs in the active normal mode subsystem, then the critical behaviour of the elastic constants will be a result of their interaction with the active normal mode. We confine our discussion to the high symmetry phase only.

The local free energy density can be written in a form similar to free energy expansion (5). As usual, the gradient term of the active normal mode amplitude is added. In the free energy density only those terms are left which describe the active normal mode j_c

and this permits us to suppress index j_c. In the hydrodynamic limit the wave-vector dependence of the expansion coefficients is disregarded.

$$F = F_0 + \tfrac{1}{2}\sum_k (\lambda + k^2) q_k q_{-k} + \tfrac{1}{2}\sum_\alpha c_\alpha \sum_k s_\alpha(k) s_\alpha(-k)$$
$$+ \tfrac{1}{2}\sum_\alpha L_\alpha \sum_{k_1 k_2} s_\alpha(k_1) q_{k_2} q_{-k_1-k_2} + \tfrac{1}{2}\sum_{\alpha\beta} K_{\alpha\beta} \sum_{k_1 k_2} s_\alpha(k_1) s_\beta(k_2) q_{-k_1-k_2}$$
$$+ \tfrac{1}{24} B \sum_{k_1 k_2 k_3} q_{k_1} q_{k_2} q_{k_3} q_{-k_1-k_2-k_3}, \tag{26}$$

where $s_\alpha(k)$ and q_k specify the fluctuations in the system.

Using the Wilson-type approach we can construct a renormalization-group transformation by integrating over intermediate wave vectors in the domain $b^{-1} < k < 1$ and making an appropriate change of scale

$$k = b^{-1}k', \quad q_k = \zeta_q q'_{k'},$$
$$s_\alpha(k) = \zeta_s s'_\alpha(k'). \tag{27}$$

The equations have been constructed by making a diagramatic expansions in the analogous to the renormalization group used by Bergman and Halperin [9]. Taking into account the diagrams up to the second order, we get the following recursion relation for λ and the normal elastic constant c_α

$$\lambda_{l+1} + k'^2 = \zeta_q^2 b^{-d}\left[\lambda_l + k^2 + \tfrac{1}{2} B_l T \sum_p \frac{1}{1+p^2}\right],$$

$$c_\alpha^{l+1} = \zeta_s^2 b^{-d}\left[c_\alpha^l - T(L_\alpha^l)^2 \sum_p \frac{1}{(\lambda_l + p^2)(\lambda_l + (k+p)^2)}\right], \tag{28}$$

where $|p|$ and $|k+p|$ are restricted to lie between b^{-1} and 1. The scale factors should satisfy $\zeta_q^2 b^{-d-2} = 1$ and $\zeta_s^2 b^{-d} = 1$. This choice ensure that the wave vector k^2 in the first equation of (28) disappears and that the elastic constants are not renormalized, provided $L_\alpha^0 = 0$.

Similarly, we can derive recursion relations for the remaining coefficients and convert them into the form of differential equations. In the second order of the perturbation theory, we find

$$\frac{d\lambda}{dl} = 2\lambda + \tfrac{1}{2} TB \frac{N}{\lambda+1}, \tag{29}$$

$$\frac{dL_\alpha}{dl} = \left(2 - \frac{d}{2}\right) L_\alpha - TL_\alpha B \frac{N}{(\lambda+1)^2}, \tag{30}$$

$$\frac{dc_\alpha}{dl} = -TL_\alpha^2 \frac{N}{(\lambda+1)^2}, \tag{31}$$

$$\frac{dK_{\alpha\beta}}{dl} = \left(1 - \frac{d}{2}\right) K_{\alpha\beta}, \tag{32}$$

$$\frac{dB}{dl} = (4-d)B - \tfrac{3}{2}\, TB^2 \frac{N}{(\lambda+1)^2}, \tag{33}$$

where $N(2\pi)^d$ is the surface area of the unit sphere in d dimensions. We notice that for $d = 3$ coefficients L_α do behave critically, provided their bare values do not vanish by symmetry whereas coefficients $K_{\alpha\beta}$ become irrelevant at T_c. From (31) it is possible to find the physical values of the elastic constants. Their temperature dependence can be estimated as

$$c_\alpha(t) = c_\alpha^l\Big|_{l=\ln\left(\frac{\xi(T)}{\xi_0}\right)}, \tag{34}$$

where $t = (T-T_c)/T_c$, $\xi(T)$ is the correlation length at temperature T close to T_c and ξ_0 is the value of that length at $\lambda = 1$, far from T_c. It is clear now, that unless $L_\alpha = 0$, c_α^l is a monotonic decreasing function of l which may lead to the negative value of c_α^l even though c_α^0 is positive.

TABLE III

The normal elastic constants c_α associated with the totally symmetric irreducible representation of the normal strain

Point groups G	c_α
$2/m$, m, 2	$\det\begin{pmatrix} c_{11}c_{12}c_{13}c_{15} \\ c_{12}c_{22}c_{23}c_{25} \\ c_{13}c_{23}c_{33}c_{35} \\ c_{15}c_{25}c_{35}c_{55}\end{pmatrix}$
222, $mm2$, mmm	$\det\begin{pmatrix} c_{11}c_{12}c_{13} \\ c_{12}c_{22}c_{23} \\ c_{13}c_{23}c_{33}\end{pmatrix}$
4, $\bar{4}$, $4/m$, $4mm$, 422, $\bar{4}2m$, $4/mmm$ 3, $\bar{3}$, 32, $3m$, $\bar{3}m$ 6, $\bar{6}$, $6/m$, 622, $6mm$, $\bar{6}m2$, $6/mmm$	$(c_{11}+c_{12})c_{33}-2c_{13}^2$
23, $m3$, 432, $\bar{4}3m$, $m3m$	$c_{11}+2c_{12}$

As a consequence, the system may become macroscopically unstable due to the fluctuations of the normal strains s_α which belong to the totally symmetric irreducible representation of the point group of the crystal and therefore represent a dilatation or "breathing" mode. Such instability in dilatation may lead to the first order phase transition with a finite change in volume. The normal elastic constants c_α which belong to the totally symmetric irreducible representation of a given point group and which exhibit the critical behaviour as described by (34), are listed in Table III.

Let us write equation (31) for the elastic constants in Voigh notation

$$\frac{dc_{ik}}{dl} = -TL_iL_k\frac{N}{(\lambda+1)^2}, \tag{35}$$

where we have used (14) and introduced $L_i = \sum_\alpha \sigma_i(\alpha)L_\alpha$. We see that some elastic constants decrease when the temperature approaches its critical value according to the experimental observations [3]. In Table I all the elastic constants which may show critical behaviour are marked with capital letters.

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