Spatial dispersion in the theory of elasticity, and distortion around defects in quasi-one-dimensional and quasi-two-dimensional crystals

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(Submitted 17 November 1980)
Zh. Eksp. Teor. Fiz. **81**, 277–289 (July 1981)

Static displacements and strains around bounded defects, in crystals consisting of weakly interacting atomic layers or chains, are considered. It is shown that in these crystals, the discreteness of the lattice shows up at distances $r \sim r_0 \sim d/\varepsilon^{1/2}$ that significantly exceed the interatomic distance d and depend on the small ratio ε of the elastic moduli. Allowance for the discreteness of the lattice and for the substantial bending energy of the atomic planes or chains leads to a violation of the continuous limiting law $u \sim r^{-2}$ at distances $r \lesssim r_0$ and to establishment of a different power law for the displacement $\mathbf{u}(\mathbf{r})$, with a smaller exponent, in the range of macroscopic distances $d \ll r \ll r_0$. The angular dependences of the displacement and strain fields are investigated. The elastic interaction between defects is considered, and it is shown that in the range $r \ll r_0$, the dependence of this interaction on distance and angle changes significantly, and the sign corresponds to repulsion of identical defects. Characteristics of diffuse scattering of x-ray beams and neutrons by defects in layer and chain crystals are discussed.

PACS numbers: 61.70.Ph, 62.20.Dc

The constants of interaction within chains of atoms of quasi-one-dimensional crystals (Q1C) or within atomic planes of quasi-two-dimensional crystals (Q2C) may be many times larger than the constants corresponding to interaction between the chains (planes). The resulting very pronounced anisotropy leads to characteristic peculiarities of many properties of the crystals, for example the oscillation spectrum and phonon specific heat[1] and a number of electronic properties.[2]

The static displacement fields produced by defects in Q1C and Q2C should also have interesting properties. Such properties are due to the pronounced anisotropy of the force constants and of the elastic moduli. For example, in the hexagonal Q2C graphite $c_{11}=106$, $c_{12}=18$, $c_{13}=1.5$, $c_{33}=3.6$, $c_{44}=0.4$ in units 10^{11} erg/cm^3 (Ref. 3), i.e., the elastic constants related to interaction of atoms in a single atomic plane and in different atomic planes differ by two orders of magnitude.

As is well known, the displacement field around defects bounded in all three directions decreases as $1/r^2$ at large distances r (significantly larger than the interatomic distances d and a characteristic dimension R_0 of a defect). The pronounced anisotropy of the elastic moduli and of the forces produced by defects should lead to a very strong angular dependence of the coefficient of $1/r^2$. More interesting, however, is the fact that this asymptotic dependence in Q1C and Q2C is established only at very large $r \gg r_0$, where $r_0 \sim d/\varepsilon^{1/2}$ depends on the anisotropy parameter ε and considerably exceeds d. For small R_0, there is a range of distances d, $R_0 \ll r \ll r_0$ within which there is established a different power-law dependence of the static displacement on r.

Thus under the action of defect-produced forces lying in an atomic plane of a Q2C, the atoms of this plane near the defect, at $r \ll r_0$, are displaced independently of the atoms in adjacent planes, because the weak forces of interplane interaction are insufficient to displace the latter. Thus for $r \ll r_0$, such displacements are described by the two-dimensional theory of elasticity and decrease as $1/r$. Only at appreciable distances $r \sim r_0$, under the action of added forces from atoms of the plane under consideration, do the displacements in adjacent planes become almost uniform, as they must be according to the usual three-dimensional equations of the theory of elasticity. In a similar manner, in a Q1C the longitudinal displacements of atoms of different chains, for $r \ll r_0$, are independent and are subject to the one-dimensional equation of the theory of elasticity, so that each half chain, to one or the other side of the defect, is displaced as a whole, and the displacement in this range is completely independent of the distance.[1)]

The components of defect-produced forces that act at an angle to the atomic planes of a Q2C or to the chains in a Q1C produce significant displacements, because the restoring forces due to the small elastic constants are in this case very small. For such displacements there is also a characteristic length $r_0 \gg d$. It is due to the fact that at small distances, the usual continuum approximation is inapplicable. Because of the smallness of the force constants between the weakly interacting atomic planes (chains), in the limiting passage from the atomic theory of crystals to the theory of elasticity it is impermissible, even for comparitively smooth strains, to retain only the first nonvanishing term of the expansion (which gives the small elastic constants) and is necessary to take account of higher terms, connected with the large forces of interaction within the atomic planes (chains). As follows from the results presented below, they lead to significant effects at macroscopic distances $r \lesssim r_0$ but $\gg d$, in particular to breakdown of the $1/r^2$ law and to a significantly slower change of the displacements.

A decrease of the displacements according to the $1/r^2$ law is a very general consequence of the usual equations of the theory of elasticity. The effects mentioned of violation of this law are actually a manifestation of spatial dispersion of the moduli of elasticity, which shows up with unusual sharpness in Q1C and Q2C. The indicated physical considerations lead to the result that the relation between the stress tensor $\hat{\sigma}$ and the strain tensor $\hat{u}$ is nonlocal, and in the **k** representation the elastic constant

$$\hat{c}=\hat{c}(\mathbf{k})$$

significantly depends on **k**; this dependence manifests itself at comparatively small $k\sim 1/r_0$. Only for sufficiently smooth fields is the usual local relation $\hat{\sigma}=\hat{c}\hat{u}$, with the usual macroscopic elastic-constant tensor $\hat{c}=\hat{c}(\mathbf{k}=0)$, valid. The sharp manifestation of spatial dispersion is essentially due to the fact that in Q1C and in Q2C the rigidity of the crystal, in nonuniform strain with characteristic length $\lesssim r_0$, is due to a greater degree to increase of the bending energy of the atomic planes or chains than to a change of their weak interaction energy. This fact shows up also in lattice dynamics.[1]

In consideration of the static displacements around defects in the region $r\lesssim r_0$, spatial dispersion is important, and this obviously complicates the problem. Even in the absence of such complications, the solution of the equations of the theory of elasticity for an anisotropic crystal, in direct space, is a quite complicated problem. It is considerably simpler to do the calculation by use of the method of static displacement waves, i.e., by transformation to a Fourier representation.[4-8] This method has an even greater advantage in the presence of spatial dispersion, and it will be used below. In the **k** representation, the solution of the equations of the theory of elasticity with allowance for spatial dispersion, as well as with the simple local relation $\hat{\sigma}=\hat{c}\hat{u}$, reduces to solution of simple algebraic equations. It is necessary to remember, however, that the elastic constants $\hat{c}(\mathbf{k})$ depend importantly on the length and direction of the vector **k**.

Below, the field of distortions around bounded defects in crystals with a small radius of interatomic interaction ($\sim d\ll r_0$) will be determined by the method of static-displacement waves. First, in Section 1, the amplitudes of these waves will be found; and then, in Sections 2 and 3, the displacement fields around defects in Q2C and in Q1C, respectively. Concrete calculations will be carried out for the simpler case of hexagonal crystals elastically isotropic in the hexagonal plane. But the qualitative picture obtained is basically correct also for crystals of lower symmetry, in which there appears only an additional (but not anomalously strong) angular dependence of the displacement field.

The indicated peculiarities of the displacements in the region $r\lesssim r_0$ must lead also to peculiarities of the strain field, and also of the energy of elastic interaction between defects. In particular, it is important that the sign of the energy of interaction of identical defects for $r\ll r_0$ corresponds to a repulsion between them, and its dependence on distance and on angles changes considerably. These effects also are discussed in Sections 2 and 3. The peculiarities of the displacement field and of the elastic interaction must obviously exert a considerable influence on the scattering of x-ray beams and of neutrons in Q1C and Q2C (see Section 1), and on the properties of phase transitions and of the kinetics of the occurrence of various processes in such crystals.

1. AMPLITUDES OF STATIC DISPLACEMENT WAVES

We consider first a crystal with a Bravais lattice, containing a certain number of defects of a definite type (and of a definite orientation) with dimensions $\sim d$, for example point defects or dislocation loops of very small radius. We shall define the position of a defect in the crystal by an index t (t may be interpreted as the number of the elementary cell that contains the center of the defect or the point defect itself) or by a radius vector $\mathbf{R}_t$. The distribution of defects in the crystal can be uniquely characterized by giving a number c_t, which assumes the values $c_t=1$ or 0, depending on whether a defect is present or absent at position t. On introduction of defects, the equilibrium positions of the atoms of the crystal no longer are located at sites of the ideal lattice, with radius vectors $\mathbf{R}_s$ (s is the number of the atom), and static displacements $\mathbf{u}_s$ occur with respect to the sites of the "average" crystal.

It is convenient to expand the quantities c_t and $\mathbf{u}_s$ a Fourier series:

$$c_t-c=\sum_{\mathbf{k}} c_{\mathbf{k}}\exp(-i\mathbf{k}\mathbf{R}_t),\quad \mathbf{u}_s=i\sum_{\mathbf{k}}\mathbf{u}_{\mathbf{k}}\exp(-i\mathbf{k}\mathbf{R}_s),\quad \mathbf{u}_{\mathbf{k}}=\mathbf{A}_{\mathbf{k}}c_{\mathbf{k}}. \tag{2}$$

Here c is the concentration of defects, and the summation extends over an elementary cell of the reciprocal lattice. Since the displacements are caused by defects, the amplitudes of the static displacement waves $\mathbf{u}_{\mathbf{k}}$ can be expressed in terms of the amplitudes of the fluctuational waves of defect concentration $c_{\mathbf{k}}$. For small defect concentrations, $\mathbf{u}_{\mathbf{k}}$ and $c_{\mathbf{k}}$ are related by the linear relation given in formula (2).

The displacements $\mathbf{u}_s$ are determined by the equilibrium conditions of lattice statics or by the conditions for a minimum of the free energy F, considered as a function of $\mathbf{u}_s$ and c_t. By using the harmonic approximation of the Born lattice theory and neglecting the change of the force constants on introduction of defects (for more details see Ref. 8, §6), one can write F in the form

$$F=F_0-\sum_{st} W_{sti}(c_t-c)u_{si}+{}^1/_2\sum_{ss'} V_{ss'ij}u_{si}u_{s'j}, \tag{3}$$

where the force constants V and W depend (in the approximation considered) only on the distances between s and s' or between s and t. Here and below, summation is understood over twice-occurring indices i, j, l, $m(=x, y, z)$. The quantities W_{st} have the meaning of forces exerted on atoms of the crystal by a defect.

The equilibrium conditions $\partial F/\partial u_{si}=0$ with use of (3) reduce to a system of $3N$ linear equations (N is the number of atoms). But if we substitute for c_t and $\mathbf{u}_s$ the Fourier expansions (2), then we can separate the $3N$ equations into systems of three equations, determining $\mathbf{A}_{\mathbf{k}}$ for each **k** [see the derivation of formula (6.3) in Ref. 8]:

$$Q_{\mathbf{k}ij}A_{\mathbf{k}j}=P_{\mathbf{k}i},\quad \mathbf{A}_{\mathbf{k}}=\hat{Q}_{\mathbf{k}}^{-1}\mathbf{P}_{\mathbf{k}},$$
$$Q_{\mathbf{k}ij}=\sum_{s'} V_{ss'ij}\exp(i\mathbf{k}\mathbf{R}_{ss'}),\quad P_{\mathbf{k}i}=-i\sum_{t} W_{sti}\exp(i\mathbf{k}\mathbf{R}_{st}),\quad \mathbf{R}_{ss'}=\mathbf{R}_s-\mathbf{R}_{s'}. \tag{4}$$

In the long-wave limit, the values of Q and P can be expanded in powers of $\mathbf{k}$. Since

$$\sum_{s'} V_{ss'ij}=0, \quad \sum_{s'} V_{ss'ij}R_{ss'l}=0, \quad \sum_{t} W_{sti}=0,$$

the expansion of Q begins with quadratic terms and that of P with linear. By use of the known relations between the force constants $V_{ss'ij}$ and the components of the elastic-constant tensor c_{ijlm},[9] and also the formulas for the tensor p_{ij} of force doublets produced by a defect (or for the characteristic strain L_{ij} corresponding to unit concentration of defects), it is easy to find an expression for the first nonvanishing terms of the expansions of Q and P:

$$Q^{(2)}_{\mathbf{k}im}=vk^2c_{ijlm}n_jn_l, \quad \mathbf{n}=\mathbf{k}/k, \tag{5}$$

$$P_{\mathbf{k}i}=kp_{ij}n_j; \quad p_{ij}=\sum_s W_{sti}R_{stj}=vc_{ijlm}L_{lm}. \tag{6}$$

Here v is the volume of the elementary cell. In Q1C and Q2C, the tensor p_{ij} may also be strongly anisotropic.

From formulas (4)–(6) it is seen that $\mathbf{A_k} \sim 1/k$ for small k; in ordinary crystals, with elastic anisotropy parameters ~ 1, the long-wave approximation is applicable over the whole range $k \ll \pi/d \sim k_m$. But in Q2C or Q1C, allowance for the quadratic terms (5) in the expansion of Q turns out to be insufficient even at comparatively small k, and it is necessary to take account of terms of the fourth order. Thus in Q2C, if the interaction between atoms of different layers, perpendicular to the Z axis, is much smaller than the interaction within layers, then the values of $Q^{(2)}_{\mathbf{k}zi}$ are determined by small elastic constants and are much smaller than $Q^{(2)}_{\mathbf{k}ij}$ with $i=x, y$; $j=x, y$. But the fourth-order terms in the expansion of $Q_{\mathbf{k}zz}$ are due specifically to the large force constants $V_{ss'zz}$ for pairs of atoms s, s' within a layer, and therefore in layered crystals they must be taken into account along with $Q^{(2)}_{\mathbf{k}zz}$, even at small k:

$$Q_{\mathbf{k}zz}=Q^{(2)}_{\mathbf{k}zz}+vc_{11}\mu k_1^4, \quad \mu=\frac{1}{24vc_{11}}\sum_{s'} V_{ss'zz}\left(\frac{\mathbf{kR}_{ss'}}{k_1}\right)^4 \sim\left(\frac{d}{\pi}\right)^2 \sim k_m^{-2}. \tag{7}$$

Here $\mathbf{k}_1$ is the projection of the vector $\mathbf{k}$ on the plane of a layer ($\mathbf{k}_1 \perp Z$). The main contribution to the sum over s' comes from terms for which $V_{ss'zz}$ are large, i.e., s and s' lie in the same plane ($\mathbf{R}_{ss'} \perp Z$). The estimate given for the parameter μ is correct if the radius of interaction $\sim d$.[2)] From symmetry considerations it follows that $V_{ss'xz}=V_{ss'yz}=0$ when $\mathbf{R}_{ss'} \perp Z$; that is, in $Q_{\mathbf{k}xz}$ and $Q_{\mathbf{k}}$ $Q_{\mathbf{k}yz}$ the terms containing k^4 are small when $k \ll k_m$.

In similar manner, in Q1C consisting of weakly interacting chains parallel to the Z axis it is necessary to take account of terms $\sim k^4$ in $Q_{\mathbf{k}ij}$ with $i,j \neq z$:

$$Q_{\mathbf{k}ij}=Q^{(2)}_{\mathbf{k}ij}+vc_{33}\mu k_z^4\delta_{ij},$$

$$\mu=\frac{1}{24vc_{33}}\sum_{s'} V_{ss'ij}\left(\frac{\mathbf{kR}_{ss'}}{k_z}\right)^4 \sim\left(\frac{d}{\pi}\right)^2 \quad (i,j\neq z). \tag{8}$$

Here the main contribution to the sum over s' comes from terms with $\mathbf{R}_{ss'} \parallel Z$. Formulas (7) and (8) take into account corrections to the theory of elasticity due to dependence of the elastic constants $c_{ijlm}(\mathbf{k})$ on $\mathbf{k}$, i.e., to spatial dispersion.

In crystals with several (ν) atoms in the elementary cell, the coefficients $A_{\mathbf{k}\gamma}$ for different sublattices γ are different, and the equations of type (4) form a system of 3ν equations. But it can be shown that in crystals with a center of inversion (not necessarily located at a site of the lattice), for small k, for calculation of the amplitudes of the displacements of the centers of gravity of the cells $\mathbf{A_k}$ it is possible, as before, to use equation (4), in which the expressions (5) of the theory of elasticity or the expressions (7) and (8), which take account of spatial dispersion, are valid for $Q_{\mathbf{k}ij}$. It must only be borne in mind that the last expressions, in the general case of many-atom crystals, are exact only if one of the two terms in the sum for $Q_{\mathbf{k}ij}$ considerably exceeds the other. If, however, both terms are of the same order of magnitude, then in the general case formulas (7) and (8) must be regarded as interpolation formulas. Only in crystals of a definite symmetry (when the sites are centers of inversion for the layers or chains and when $Q_{\mathbf{k}ij}$ and μ for different layers or chains are the same) are these formulas exact, as they are in one-atom crystals. Formulas (2)–(8) may be applied also to nonideal crystals with several types of defects, since in the linear theory the displacements produced by them combine additivity.

We note that for large displacements of the atoms in the crystals considered, effects due to higher-order terms in the expansion (3) in powers of the displacements may be important. In this case, we may include in the defect a certain number of greatly displaced atoms of the crystal, and we may interpret p_{ij} as the force-doublet tensor produced by such a generalized defect.

In hexagonal crystals, the elastic properties are isotropic in the plane perpendicular to the sixth-order axis Z, and in (7) the coefficient μ is independent of the direction of the vector $\mathbf{k}_1$. As a result, for defects possessing axial symmetry, the system of three equations (4) reduces to a simpler system of two equations, which determine $\mathbf{A}_{\mathbf{k}z}$ and the projection $\mathbf{A}_{\mathbf{k}1}=\mathbf{n}_1A_{\mathbf{k}1}$ ($\mathbf{n}_1=\mathbf{k}_1/k$) of the vector $\mathbf{A_k}$ on the XY plane (see Appendix II in Ref. 8). For Q2C, these equations, with use of (5)–(7), have the form

$$\begin{aligned}&(c_{11}k_1^2+c_{44}k_z^2)A_{\mathbf{k}1}+(c_{13}+c_{44})k_1k_zA_{\mathbf{k}z}=\frac{1}{v}p_{xx}k_1,\\&(c_{13}+c_{44})k_1k_zA_{\mathbf{k}1}+(c_{44}k_1^2+c_{33}k_z^2+c_{11}\mu k_1^4)A_{\mathbf{k}z}=\frac{1}{v}p_{zz}k_z,\end{aligned} \tag{9}$$

and their solution is

$$\begin{gathered}\mathbf{A}_{\mathbf{k}1}=A_{\mathbf{k}1}\mathbf{n}_1, \quad A_{\mathbf{k}1}=\frac{k_1}{D}[p_1(\varepsilon_1k_1^2+\varepsilon_3k_z^2+\mu k_1^4)-p_3\varepsilon_2k_z^2],\\ A_{\mathbf{k}z}=\frac{k_z}{D}[p_3(k_1^2+\varepsilon_1k_z^2)-p_1\varepsilon_2k_1^2],\\ p_1=\frac{p_{xx}}{vc_{11}}, \quad p_3=\frac{p_{zz}}{vc_{11}}, \quad \varepsilon_1=\frac{c_{44}}{c_{11}}, \quad \varepsilon_2=\frac{c_{13}+c_{44}}{c_{11}}, \quad \varepsilon_3=\frac{c_{33}}{c_{11}},\\ D=(k_1^2+\varepsilon_1k_z^2)(\varepsilon_1k_1^2+\varepsilon_3k_z^2+\mu k_1^4)-\varepsilon_2^2k_1^2k_z^2.\end{gathered} \tag{10}$$

In Q1C, in accordance with (8), in the first equation (9) a term $c_{33}\mu k_z^4A_{\mathbf{k}l}$ appears, and in the second the term $c_{11}\mu k_1^4A_{\mathbf{k}z}$ disappears. The solution of the resulting system has the form

$$A_{\mathbf{k}1}=\frac{k_1}{D}\left[p_1(k_z^2+\varepsilon_1 k_1^2)-p_3\varepsilon_2 k_z^2\right],$$

$$A_{\mathbf{k}z}=\frac{k_z}{D}\left[p_3(\varepsilon_3 k_1^2+\varepsilon_1 k_z^2+\mu k_z^4)-p_1\varepsilon_2 k_1^2\right],$$

$$p_1=\frac{p_{xx}}{vc_{33}},\quad p_3=\frac{p_{zz}}{vc_{33}},\quad \varepsilon_1=\frac{c_{44}}{c_{33}},\quad \varepsilon_2=\frac{c_{13}+c_{44}}{c_{33}},\quad \varepsilon_3=\frac{c_{11}}{c_{33}},$$

$$D=(k_z^2+\varepsilon_1 k_1^2)(\varepsilon_3 k_1^2+\varepsilon_1 k_z^2+\mu k_z^4)-\varepsilon_2^2 k_1^2 k_z^2. \tag{11}$$

In Q2C the constants c_{33}, c_{44}, and c_{13} are small in comparison with c_{11}; and in Q1C, c_{11}, c_{44}, and c_{13} are small in comparison with c_{33}. Therefore ε_1, ε_2, and ε_3 (which, like μ, p_1, and p_3, have different meanings in Q1C and in Q2C) are dimensionless small parameters. According to (10) and (11), in hexagonal crystals $\mathbf{A_k}$ depends only on the angle θ between $\mathbf{k}$ and the Z axis.

The amplitudes $\mathbf{A_k}$ of the displacement waves have direct physical meaning; in particular, they determine the intensity of the diffuse scattering caused by the distortions,

$$I_1(\mathbf{K}+\mathbf{k})\sim(\mathbf{K}\mathbf{A_k})^2$$

in the vicinity of sites of the reciprocal lattice (with reciprocal-lattice vectors $\mathbf{K}$). It is evident from (10) that when $|p_1|\sim|p_3|$ and $\varepsilon_1\sim\varepsilon_2\sim\varepsilon_3$, as $k\to 0$ in Q2C, $A_{\mathbf{k}1}$ increases as $1/k$ and depends very strongly on angles, varying as

$$A_{\mathbf{k}1}\approx\left(p_1-p_3\frac{\varepsilon_2}{\varepsilon_1}\right)\frac{1}{k}\frac{\theta}{\theta^2+\varepsilon_1}\qquad(\theta\lesssim\varepsilon_1^{1/2})$$

in the range of very small θ. The component

$$A_{\mathbf{k}z}\approx\frac{p_3 k_z}{\varepsilon_1 k_1^2+\varepsilon_3 k_z^2+\mu k_1^4}\qquad(|p_3|\gg|p_1|\varepsilon_2)$$

is very large at small k (where $|A_{\mathbf{k}z}|\sim(\varepsilon k)^{-1}\gg|A_{\mathbf{k}1}|$). But at comparatively small

$$k\sim\left(\frac{\varepsilon}{\mu}\right)^{1/2}\frac{1}{\theta}\sim\frac{\varepsilon^{1/2}k_m}{\theta}\ll k_m$$

(outside the small-θ range), spatial dispersion leads to a significant decrease of $|A_{\mathbf{k}z}|$ and to a change of its law of decrease with increase of k: $A_{\mathbf{k}z}\sim k^{-3}$. Accordingly, in this range the diffuse scattering is found to be significantly suppressed (I_1 decreases as k^{-6}, instead of the usual Huang law k^{-2}). If, in Q2C, $|p_1|\gg|p_3|$ and $|p_1|\varepsilon_2\gtrsim|p_3|$, then $A_{\mathbf{k}z}$ is determined by the general formula (10).

In Q1C with $|p_1|\sim|p_3|$ and $\varepsilon_1\sim\varepsilon_2\sim\varepsilon_3$,

$$A_{\mathbf{k}1}\approx\frac{p_1 k_1}{\varepsilon_3 k_1^2+\varepsilon_1 k_z^2+\mu k_z^4},$$

$$A_{\mathbf{k}z}\approx\left(p_3-p_1\frac{\varepsilon_2 k_1^2}{\varepsilon_3 k_1^2+\varepsilon_1 k_z^2+\mu k_z^4}\right)\frac{k_z}{k_z^2+\varepsilon_1 k_1^2}$$

and $|A_{\mathbf{k}1}|\gg|A_{\mathbf{k}z}|$ (except in the small-θ range). Here the spatial dispersion strongly diminishes $A_{\mathbf{k}1}$ and leads to the relation

$$A_{\mathbf{k}1}\approx p_1\frac{k_1}{\mu k_z^4}\sim\frac{1}{k^3}\quad\text{when }k\cos\theta\gg\left(\frac{\varepsilon}{\mu}\right)^{1/2}\sim\varepsilon^{1/2}k_m.$$

This picture of characteristic strong dependence of $\mathbf{A_k}$ on $\mathbf{k}$, as follows from (4)–(8), remains valid also in Q1C or Q2C of lower symmetry. But in contrast to hexagonal crystals, now $\mathbf{A_k}$ depends not only on θ but also on the direction of $\mathbf{k}_1$ in the plane perpendicular to the distinguished axis.

2. QUASI-TWO-DIMENSIONAL CRYSTALS

With the aid of the expressions given for $\mathbf{A_k}$, it is not difficult to find also the displacements $\mathbf{u}_s$ around an individual defect. Let the center of the defect be located at the origin of coordinates. Then $c_t=1$ only when $\mathbf{R}_t=0$, and $c_\mathbf{k}=N^{-1}$; the Fourier expansion (2), in crystals with a Bravais lattice, takes the form

$$\mathbf{u}_s=\mathbf{u}(\mathbf{r})=\frac{v}{8\pi^3}\int d\mathbf{k}\mathbf{A_k}\sin\mathbf{kr}, \tag{12}$$

where $\mathbf{r}=\mathbf{R}_s$ and where the integration extends over the volume of an elementary cell of the reciprocal lattice. In the range $r\gg d$, with neglect of corrections $\sim d/r$ [or $(d/r)^2$ in the presence of a center of inversion], formula (12) is applicable also to crystals with several atoms in a cell.

In the limit $r\to\infty$, the main contribution to the integral (12) comes from the region $k\to 0$, and $\mathbf{u}(\mathbf{r})\sim 1/r^2$ is determined by the asymptotic expression[7]

$$\mathbf{u}(\mathbf{r})=\frac{v}{8\pi^2r^2}\lim_{k\to 0,\ n_\mathbf{r}\to 0}\int_0^{2\pi}d\psi\frac{\partial(k\mathbf{A_k})}{\partial n_r}\qquad(r\to\infty), \tag{13}$$

where n_r is the projection of $\mathbf{n}=\mathbf{k}/k$ on the axis $\mathbf{r}$, and where the integration over ψ extends over directions of $\mathbf{n}$ perpendicular to $\mathbf{r}$. But in the cases of Q2C and Q1C under consideration, the dependence of $k\mathbf{A_k}$ on $\mathbf{k}$ produced by spatial dispersion leads to a more complicated $\mathbf{u}(\mathbf{r})$ relation in the range $d\varepsilon^{-1/2}\gg r\gg d$.

In order to illustrate effects due to spatial dispersion, we consider hexagonal Q2C. Excluding at first the case of small r, we may extend the region of integration in (12) over all space and determine $\mathbf{A_k}$ by formula (10). Using cylindrical coordinates k_1, φ, k_z, which are convenient in this case, and carrying out the integration over φ ($A_{\mathbf{k}1}$ and $A_{\mathbf{k}z}$ are independent of φ), we express $\mathbf{u}(\mathbf{r})$ in the form

$$\mathbf{u}_1(\mathbf{r})=u_1(\mathbf{r})\mathbf{e}_1,\quad u_1=\frac{v}{4\pi^2}\int_{-\infty}^{\infty}\int_0^{\infty}dk_z dk_1 k_1 A_{\mathbf{k}1}J_1(k_1r_1)\cos k_z z,$$

$$u_z(\mathbf{r})=\frac{v}{4\pi^2}\int_{-\infty}^{\infty}\int_0^{\infty}dk_z dk_1 k_1 A_{\mathbf{k}z}J_0(k_1r_1)\sin k_z z. \tag{14}$$

Here u_z, z, $\mathbf{u}_1$, and $\mathbf{r}_1$ are the projections of $\mathbf{u}$ and $\mathbf{r}$ on the hexagonal axis and on the plane perpendicular to it, $\mathbf{e}_1=\mathbf{r}_1/r_1$ is a unit vector in this plane, and $J_\nu(x)$ is the Bessel function of order ν.

In the case of small ε under consideration, one can expand $1/D$ in formulas (10) in powers of ε_2^2 and truncate after the linear term of the expansion [in the integration of the zero-order term of the expansion, the rapidly oscillating function $J_1(k_1r_1)$ may lead to a compensation that sharply decreases the integral and necessitates taking the linear term into account]. After this, the integrals (14) over k_z are carried out explicitly; and with neglect of terms of higher order in ε_1 and ε_2 (but not in $p_1\varepsilon/p_3$), the expressions for u_1 and u_z take the form

$$u_1(\mathbf{r})=\frac{v}{4\pi}\int_0^{\infty}dk_1\,k_1J_1(k_1r_1)\left[\frac{P_1}{\varepsilon_1^{1/2}}\exp\left(-\frac{k_1|z|}{\varepsilon_1^{1/2}}\right)\right.$$
$$\left.+\frac{P_3\varepsilon_2}{\varepsilon_3^{3/2}}(\varepsilon_1+\mu k_1^2)^{1/2}\exp\left\{-\left(\frac{\varepsilon_1+\mu k_1^2}{\varepsilon_3}\right)^{1/2}k_1|z|\right\}\right], \tag{15}$$

$$u_z(\mathbf{r})=\frac{v}{4\pi}\frac{z}{|z|}\int_0^\infty dk_1\,k_1J_0(k_1r_1)\left[\frac{P_3}{\varepsilon_3}\exp\left\{-\left(\frac{\varepsilon_1+\mu k_1^2}{\varepsilon_3}\right)^{1/2}k_1|z|\right\}\right.$$
$$\left.+\frac{P_1\varepsilon_2}{\varepsilon_3}\exp\left\{-\frac{1}{\varepsilon_1^{1/2}}k_1|z|\right\}\right],\quad P_1=p_1-p_3\frac{\varepsilon_2}{\varepsilon_3},\quad P_3=p_3-p_1\varepsilon_2.$$

At sufficiently large r, the main contribution to the integrals in (15) comes from the small $-k_1$ range, in which μk_1^2 may be neglected along with ε_1, and

$$\mathbf{u}_1(\mathbf{r})=\frac{v}{4\pi}\left[P_1\varepsilon_1^{1/2}\frac{\varepsilon_1^{1/2}r_1}{(z^2+\varepsilon_1r_1^2)^{3/2}}+P_3\varepsilon_2\frac{\varepsilon_1^{1/2}r_1}{(\varepsilon_1z^2+\varepsilon_3r_1^2)^{3/2}}\right]\mathbf{e}_1,$$
$$u_z(\mathbf{r})=\frac{v}{4\pi}\left[P_3\frac{\varepsilon_1^{1/2}z}{(\varepsilon_1z^2+\varepsilon_3r_1^2)^{3/2}}+P_1\frac{\varepsilon_1\varepsilon_2}{\varepsilon_3}\frac{z}{(z^2+\varepsilon_1r_1^2)^{3/2}}\right]\tag{16}$$
$$(r_1\gg d'/\varepsilon_1^{1/2}\quad\text{or}\quad z\gg\varepsilon_3^{1/2}d'/\varepsilon_1),\quad d'=\mu^{1/2}\sim d.$$

In agreement with (13), in the large $-r$ range $\mathbf{u}(\mathbf{r})\sim1/r^2$, and $|u_z|\gg|u_1|$ (except for the case of very small $|z|/r$). Similar numerical calculations of the displacement and strain fields around dislocation loops in the Q2C graphite (without allowance for spatial dispersion) were made in a paper of Ohr.[11]

At smaller $r\sim d'/\varepsilon^{1/2}$, it is not permissible in the expressions (15) to neglect the terms μk_1^2 along with ε_1, i.e., to neglect the spatial dispersion. In this range, it is not difficult to find u_z and u_1 by carrying out a numerical integration in (15). But if $r\ll d'/\varepsilon^{1/2}$, then the integrals in (15) can be calculated analytically:

$$\mathbf{u}_1(\mathbf{r})=\frac{v}{16\pi}\frac{P_3\varepsilon_2}{(\mu\varepsilon_3)^{1/2}}\left[\frac{r_1}{z^2}e^{-a}+\frac{2\varepsilon_1}{\varepsilon_3}\frac{1}{r_1}(1-e^{-a})\right.$$
$$\left.-\frac{\varepsilon_1^2r_1}{4\mu\varepsilon_3}\ln\frac{4.8\mu^{1/2}}{\varepsilon_1^{1/2}(r_1+\zeta|z|)}\right]\mathbf{e}_1+\frac{v}{4\pi}P_1\varepsilon_1\frac{r_1}{z^3}\mathbf{e}_1,$$
$$u_z(\mathbf{r})=\frac{v}{8\pi}\frac{P_3}{(\mu\varepsilon_3)^{1/2}}\left[\frac{1}{z}\left(1-\frac{1}{2}\frac{\varepsilon_1z}{(\mu\varepsilon_3)^{1/2}}\right)e^{-a}\right.\tag{17}$$
$$\left.+\frac{\varepsilon_1^2z}{4\mu\varepsilon_3}\ln\frac{1.75\mu^{1/2}}{\varepsilon_1^{1/2}(r_1+\zeta|z|)}\right]+\frac{v}{4\pi}P_1\frac{\varepsilon_1\varepsilon_2}{\varepsilon_3}\frac{1}{z^2},$$
$$a=\frac{\varepsilon_3^{1/2}}{4\mu^{1/2}}\frac{r_1^2}{|z|}\sim\frac{r_1^2\varepsilon^{1/2}}{d'|z|},\quad\zeta\sim\left(\frac{\varepsilon_1}{\varepsilon_3}\right)^{1/2}\left(d\ll|z|\ll\frac{(\varepsilon_3\mu)^{1/2}}{\varepsilon_1}\sim\frac{d'}{\varepsilon^{1/2}},d\ll r_1\ll\frac{d'}{\varepsilon_1^{1/2}}\right).$$

In the range $a\lesssim1$ ($r_1^2\lesssim|z|d'/\varepsilon^{1/2}$), the larger component u_z is

$$u_z=\frac{v}{8\pi}\frac{P_3}{(\mu\varepsilon_3)^{1/2}}\frac{1}{z}e^{-a}.\tag{18}$$

Thus with approach to the defect, the displacements u_z increase considerably more slowly at a distance $\sim d'/\varepsilon^{1/2}$ than at larger distances, and for $|z|\ll d'/\varepsilon^{1/2}$, $a\ll1$ they vary as $1/z$. We note that in the range under consideration, namely $|z|\ll d'/\varepsilon^{1/2}$, when $r_1\sim|z|$, then always $a\ll1$, and formulas (17), (19), and (20) simplify. Similarly, on passage into this range the increase of the strain slows down (from a $1/r^3$ law to a $1/z^2$ law), as does that of the energy of elastic interaction of the defects. Thus, for example, the large components of the strain tensor, u_{zz} and u_{zr_1}, are according to (16) and (17) determined by the expressions

$$u_{zr_1}=-\frac{3v}{8\pi}P_3\frac{\varepsilon_1^{1/2}\varepsilon_3zr_1}{(\varepsilon_1z^2+\varepsilon_3r_1^2)^{5/2}}-\frac{3v}{8\pi}P_1\frac{\varepsilon_1zr_1}{(z^2+\varepsilon_1r_1^2)^{5/2}},$$
$$u_{zz}=\frac{v}{4\pi}P_3\varepsilon_1\frac{\varepsilon_3r_1^2-2\varepsilon_1z^2}{(\varepsilon_1z^2+\varepsilon_3r_1^2)^{5/2}}-\frac{v}{4\pi}P_1\frac{\varepsilon_1\varepsilon_2}{\varepsilon_3}\frac{2z^2-\varepsilon_1r_1^2}{(z^2+\varepsilon_1r_1^2)^{5/2}}\quad\left(r\gg\frac{d'}{\varepsilon^{1/2}}\right),\tag{19}$$
$$u_{zr_1}=-\frac{v}{32\pi}\frac{P_3}{\mu}\frac{r_1}{z|z|}e^{-a},$$
$$u_{zz}=-\frac{v}{8\pi}\frac{P_3}{(\mu\varepsilon_3)^{1/2}}\frac{1}{z^2}(1-a)e^{-a}\quad(d\ll r\ll d'/\varepsilon^{1/2},\ a\leqslant1).$$

The energy E of elastic interaction of the defect under consideration with another defect, with force-doublet tensor p_{ij}', in the case when $|p_3|\gg|p_1|\varepsilon$ and $|p_3'|\gg|p_1'|\varepsilon$, has the form, by use of (18) and (19),

$$E(\mathbf{r})=-p_{ij}'u_{ij}(\mathbf{r})=\frac{v^2}{4\pi}c_{11}p_3p_3'\varepsilon_1^{1/2}\frac{2\varepsilon_1z^2-\varepsilon_3r_1^2}{(\varepsilon_1z^2+\varepsilon_3r_1^2)^{5/2}}$$
$$(r\gg d'/\varepsilon^{1/2},\quad z^2\gg\varepsilon^{4/3}(p_1p_1'/p_3p_3')^{2/3}r_1^2,\quad z^2\gg\varepsilon r_1^2),\tag{20}$$
$$E(\mathbf{r})=\frac{v^2}{8\pi}c_{11}\frac{p_3p_3'}{(\mu\varepsilon_3)^{1/2}}\frac{1}{z^2}(1-a)e^{-a}$$
$$\left(\frac{d'}{\varepsilon^{1/2}}\gg|z|\gg\frac{d'}{\varepsilon^{1/2}}\left|\frac{p_1p_1'}{p_3p_3'}\right|\varepsilon^2e^a\right).$$

It is important that on approach of the defects to each other along a straight line at a given angle θ' to the Z axis, the interaction energy changes sign in the range $r\sim d'/\varepsilon^{1/2}$, if $(z/r_1)^2>2\varepsilon_1/\varepsilon_3$ and $r_1\sim|z|$. Over almost the whole region $r\ll d'/\varepsilon^{1/2}$ (except, perhaps, a small section with $\theta'\approx\pi/2$), the sign of E corresponds to repulsion of identical defects. The dependences of the energy on r and on the angles for $r\gg d'/\varepsilon^{1/2}$ and for $r\ll d'/\varepsilon^{1/2}$ differ significantly.

The displacement field in the plane $z=0$ of a Q2C and in neighboring planes requires special treatment. In this range, an important contribution to the integral (12) for $\mathbf{u}_1(\mathbf{r})$ is made by large $k_z\sim k_m$, where the longwave approximation (10) is invalid and it is necessary to determine $\mathbf{A}_\mathbf{k}$ from the general equations of the type (4). We separate $\mathbf{A}_\mathbf{k}=\mathbf{A}_\mathbf{k}^0+\varepsilon\mathbf{A}_\mathbf{k}'$ for $k_1^2\gg\varepsilon_1k_m^2$ into a term $\mathbf{A}_\mathbf{k}^0$, corresponding to displacements within the atomic plane under consideration (perpendicular to Z) and with neglect of the interaction between planes, and a term $\varepsilon\mathbf{A}_\mathbf{k}'$, which takes this interaction into account. The value of $\mathbf{A}_\mathbf{k}^0=\mathbf{A}_\mathbf{k}^0(\mathbf{k}_1)$ is determined by the two equations (4) with $i=x,y$ for $\varepsilon=0$ (or by the analogous system of equations for crystals with several atoms in a cell) and depends only on $\mathbf{k}_1$, whereas $\mathbf{A}_\mathbf{k}'$, depends both on $\mathbf{k}_1$ and on k_z and is determined by the complete system (4). When $k_1\ll k_m$, we may pass to the macroscopic limit in the equations for $\mathbf{A}_\mathbf{k}^0$; each atomic layer z (z is a multiple of the interplane distance d_z) must be characterized by its own force-doublet tensor

$$p_{ij}^z=\sum_s{}^{(z)}W_{sti}R_{stj},$$

determined by the forces $\mathbf{W}_{st}$ with which the defect acts on the atoms of this plane. In hexagonal crystals, for $k_1\ll k_m$, in analogy to (10), $\mathbf{A}_\mathbf{k}^0(\mathbf{k}_1,z)=p_1^z\mathbf{k}_1/k_1^2$, where $p_1^z=p_{xx}/vc_{11}$. On substituting this expression in (12) and taking into account that the integral $\int\cos k_zz\,dk_z=2\pi/d_z$ when $z=0$ and $=0$ when $z\neq0$, we find that the displacements u_1^z of the atoms of plane z and $E(\mathbf{r})$ in the zero-order approximation with respect to ε are determined by the formulas

$$\mathbf{u}_1^z(\mathbf{r})=\frac{v}{2\pi d_z}p_1^z\frac{\mathbf{r}_1}{r_1^2},\quad E(\mathbf{r})=\frac{v^2c_{11}}{2\pi d_zr_1^2}\sum_z p_1^zp_1'^z\quad\left(d\ll r_1\ll\frac{d}{\varepsilon_1^{1/2}}\right).\tag{21}$$

From (21) it is evident that for $z=0$ and for values of z less than the dimension R_0 of the defect and its radius r^0 of interaction with atoms of the crystal (where $p_1^z\neq0$), and for $r_1\ll d/\varepsilon^{1/2}$, the displacements vary according to the law $u_1\sim1/r$ characteristic of two-dimensional crystals. In the range $r_1\gtrsim d/\varepsilon_1^{1/2}$, the displacements are determined by values of $\mathbf{A}_\mathbf{k}$ at small $k_1<\varepsilon_1^{1/2}k_m$, where, as is evident from (10), neglect of terms $\sim\varepsilon_1k_z^2$ along with

k_1^2 becomes incorrect, and the relation (21) breaks down, transforming for $r_1 \gg d/\varepsilon_1^{1/2}$ to the relation (16) for $\mathbf{u}_1(\mathbf{r})$. When $|z| > R_0$, r^0, $r_1 \ll d/\varepsilon_1^{1/2}$: (21) vanishes, and the displacements are determined by $\varepsilon \mathbf{A}_\mathbf{k}'$; that is, in contrast to (21), they contain the small factor ε. In Q2C of lower symmetry, the field $u_1^z(\mathbf{r}_1)$ for small z and for $r_1 \ll d/\varepsilon^{1/2}$ is not isotropic, but as before it varies as $1/r_1$.

3. QUASI-ONE-DIMENSIONAL CRYSTALS

In calculating the displacements in hexagonal Q1C at not too small r, it is possible to determine $\mathbf{A}_\mathbf{k}$ from formula (11) and to extend the integration in (12) over all space. Then u_1 and u_z are determined by formulas (14). As in the case of Q2C, we expand $1/D$ in (11) in powers of ε_2^2 and truncate after the linear terms. This enables us to carry out the integration over k_1 in (14) and to reduce the expressions for u_1 and u_z to one-variable integrals. With neglect of terms of higher order in ε (but not in $p_3\varepsilon/p_1$), they have the form

$$\mathbf{u}_1(\mathbf{r}) = \frac{v}{2\pi^2}\int_0^\infty dk_z\,k_z\cos k_z z\left\{P_1\frac{1}{\varepsilon_3}(\varepsilon_1+\mu k_z^2)^{1/2}K_1\left[\left(\frac{\varepsilon_1+\mu k_z^2}{\varepsilon_3}\right)^{1/2}k_z r_1\right]\right.$$
$$\left.+P_3\frac{\varepsilon_2}{\varepsilon_3\varepsilon_1^{1/2}}K_1\left(\frac{k_z r_1}{\varepsilon_1^{1/2}}\right)\right\}\mathbf{e}_1;$$
$$u_z(\mathbf{r}) = \frac{v}{2\pi^2}\int_0^\infty dk_z\,k_z\sin k_z z\left\{P_3\frac{1}{\varepsilon_1}K_0\left(\frac{k_z r_1}{\varepsilon_1^{1/2}}\right)+P_1\frac{\varepsilon_2}{\varepsilon_3^2}(\varepsilon_1+\mu k_z^2)\right.$$
$$\left.\times K_0\left[\left(\frac{\varepsilon_1+\mu k_z^2}{\varepsilon_3}\right)^{1/2}k_z r_1\right]\right\},\quad P_1 = p_1 - p_3\varepsilon_2,\quad P_3 = p_3 - p_1\frac{\varepsilon_2}{\varepsilon_3}, \tag{22}$$

where $K_\nu(x)$ [and, below, $I_\nu(x)$] are modified Bessel functions.

At large r, neglecting μk_z^2 in comparison with ε_1, we get

$$u_1(\mathbf{r}) = \frac{v}{4\pi}\left[P_1\left(\frac{\varepsilon_1}{\varepsilon_3}\right)^{1/2}\frac{\varepsilon_1 r_1}{(\varepsilon_1 r_1^2+\varepsilon_3 z^2)^{3/2}}+P_3\frac{\varepsilon_2\varepsilon_1^{1/2}}{\varepsilon_3}\frac{r_1}{(r_1^2+\varepsilon_1 z^2)^{3/2}}\right]\mathbf{e}_1,$$
$$u_z(\mathbf{r}) = \frac{v}{4\pi}\left[P_3\frac{\varepsilon_1 z}{(r_1^2+\varepsilon_1 z^2)^{3/2}}+P_1\frac{\varepsilon_1\varepsilon_2}{\varepsilon_3}\frac{\varepsilon_3 z}{(\varepsilon_1 r_1^2+\varepsilon_3 z^2)^{3/2}}\right] \tag{23}$$
$$(r_1 \gg (\mu\varepsilon_3)^{1/2}/\varepsilon_1 \sim d'/\varepsilon^{1/2}\quad\text{or}\quad |z| \gg d'/\varepsilon_1^{1/2}).$$

In Q1C, the large components of the displacement vector are those in the plane perpendicular to the chains ($|u_1| \gg |u_z|$ outside the region of very small θ').

When $r \sim d'/\varepsilon^{1/2}$, it is necessary to take into account terms μk_z^2 in the expressions (22). In the range $r \ll d'/\varepsilon^{1/2}$, with neglect of ε_1 together with μk_z^2, the resulting integral for the larger component u_1 of the displacement vector can be calculated analytically:

$$\mathbf{u}_1(\mathbf{r}) = \frac{v}{16\pi}\frac{P_1}{(\mu\varepsilon_3)^{1/2}}\frac{|z|}{r_1^2}\left[f(b)+b\frac{df(b)}{db}\right]\mathbf{e}_1+\frac{v}{4\pi}P_3\frac{\varepsilon_2\varepsilon_1^{1/2}}{\varepsilon_3 r_1^2}\mathbf{e}_1,$$
$$b = \frac{\varepsilon_3^{1/2}z^2}{8\mu^{1/2}r_1},\quad f(b) = K_{1/4}(b)\,[I_{1/4}(b)+I_{-1/4}(b)] \tag{24}$$
$$(d \ll r_1 \ll (\mu\varepsilon_3)^{1/2}/\varepsilon_1 \sim d'/\varepsilon^{1/2},\quad d \ll |z| \ll d'/\varepsilon_1^{1/2}).$$

Formula (24) can be simplified by using the limiting values of $K_\nu(b)$ and $I_\nu(b)$ at small and large b:

$$\mathbf{u}_1 = \frac{2^{1/2}v}{16\Gamma^2(3/4)}\frac{P_1}{\mu^{1/4}\varepsilon_3^{3/4}}\frac{1}{r_1^{3/2}}\mathbf{e}_1\quad(b \ll 1),$$
$$\mathbf{u}_1 = -\frac{6v}{\pi}\frac{P_1\mu}{\varepsilon_3^2}\frac{r_1}{z^5}\mathbf{e}_1-\frac{v}{15\pi^2}\frac{P_1\varepsilon_1^{5/2}}{(\mu\varepsilon_3)^{3/2}}r_1\ln\left(\frac{\zeta'(\mu\varepsilon_3)^{1/2}}{\varepsilon_1 r_1}\right)\mathbf{e}_1 \tag{25}$$
$$+\frac{v}{4\pi}\frac{P_3\varepsilon_2\varepsilon_1^{1/2}}{\varepsilon_3}\frac{1}{r_1^2}\mathbf{e}_1\quad(b \gg 1),\quad \zeta' \sim 1.$$

In the formula for $\mathbf{u}_1$ relating to the case $b \gg 1$, a term has been added that is important in this range and is proportional to $\varepsilon_1^{5/2}$ and logarithmically dependent on r_1 [it was omitted in (24)]. Terms have been omitted that differ from the first term by small factors of the type $(\varepsilon_1 z^2/d'^2 b)^n$ (for $b \gg 1$) or $(\varepsilon^{1/2}r_1/d')^n$.

In Q1C, on approach to a defect in the range $r_1 \ll d'/\varepsilon^{1/2}$, $b \ll 1$, the displacements increase as $r_1^{-3/2}$, i.e. faster than in Q2C but more slowly than at large distances. The large components of the strain tensor $u_{r_1 r_1}\ldots$ and the energy of elastic interaction of the defects for $r_1 \lesssim d'/\varepsilon^{1/2}$ also change more slowly than the usual r^{-3} law. When $|p_1| \gg |p_3|\varepsilon_2$ and $|p_1'| \gg |p_3'|\varepsilon_2$,

$$E(\mathbf{r}) \approx -vc_{33}p_1'\left(\frac{\partial u_1}{\partial r_1}+\frac{u_1}{r_1}\right) = \frac{v^2 c_{33}p_1 p_1'\varepsilon_1}{4\pi\varepsilon_3^{1/2}}\frac{\varepsilon_1 r_1^2-2\varepsilon_3 z^2}{(\varepsilon_1 r_1^2+\varepsilon_3 z^2)^{5/2}}$$
$$(r \gg d'/\varepsilon^{1/2},\quad r_1^2 \gg \varepsilon\,(p_3 p_3'/p_1 p_1')^{2/3}z^2,\quad r_1^2 \gg \varepsilon z^2), \tag{26}$$
$$E(\mathbf{r}) = \frac{2^{1/2}}{32\Gamma^2(3/4)}\frac{v^2 c_{33}p_1 p_1'}{\mu^{1/4}\varepsilon_3^{3/4}}\frac{1}{r_1^{5/2}}\quad\left(r \ll \frac{d'}{\varepsilon^{1/2}},\quad b \ll 1\right).$$

The sign of $E(\mathbf{r})$ in the range $r \ll d/\varepsilon^{1/2}$ corresponds to repulsion of the defects.

When $\mathbf{r}_1 = 0$ and at small r_1, the displacements u_1 become small, and the component u_z is the largest. To determine its value in the chain of atoms with $\mathbf{r}_1 = 0$ (containing the center of the defect) and in neighboring chains, we proceed as in the consideration of displacements near the plane $z = 0$ in Q2C, and set $\mathbf{A}_\mathbf{k} = \mathbf{A}_\mathbf{k}^0 + \varepsilon\mathbf{A}_\mathbf{k}'$, where $\mathbf{A}_\mathbf{k}^0 = \mathbf{A}_\mathbf{k}^0(k_z)$ is determined by equation (4) with $i = z$. At small k_z, for the chain $\mathbf{r}_1$

$$\mathbf{A}_\mathbf{k}^0(\mathbf{r}_1) = p_3(\mathbf{r}_1)/k_z,\quad p_{zz}(\mathbf{r}_1) = vc_{33}p_3(\mathbf{r}_1) = \sum_s^{(\mathbf{r}_1)} W_{stz}R_{stz}$$

(the summation extends only over atoms of this chain). On substituting this expression in (12) and taking into account that the integral $\int \cos\mathbf{k}_1\mathbf{r}_1 d\mathbf{k}_1 = 4\pi^2/\Delta$ for $\mathbf{r}_1 = 0$ (Δ is the area per chain in the XY plane) and when $\mathbf{r}_1 \neq 0$, we find an expression for the displacements $u_z^{\mathbf{r}_1}$ of atoms of the chain $\mathbf{r}_1$:

$$u_z^{\mathbf{r}_1}(\mathbf{r}) = \frac{v}{2\Delta}p_3(\mathbf{r}_1)\,\mathrm{sign}\,z\quad(|z| \ll d/\varepsilon_1^{1/2}). \tag{27}$$

In Q1C at small z, the defect displaces as a whole the sections of the chains that are located within its radius of interaction (in opposite directions). Only at distances $|z| \sim d/\varepsilon_1^{1/2}$ does the interaction with other chains begin to show up, gradually leading to the establishment of the $u_z \sim r^{-2}$ law described by formula (23).

For the longitudinal displacements produced by the forces W_{stz} along the chains, one can obtain also more general integral representations, correct for all $|z| \gg d'$ (larger than the radius of interatomic interaction $\sim d$). For example, when $p_1 = 0$, by substituting the solution of equation (4), $A_{\mathbf{k}z} = P_{\mathbf{k}z}Q^{-1}_{\mathbf{k}zz'}$ in the important region $|k_z| \ll k_1 \lesssim k_m$ in (12), one finds that

$$u_z(\mathbf{r}) = \frac{v}{8\pi^2}\sum_{\mathbf{r}_1'}p_3(\mathbf{r}_1')\int d\mathbf{k}_1\cos\mathbf{k}_1(\mathbf{r}_1-\mathbf{r}_1')\exp\left[-(\varepsilon\varphi(\mathbf{k}_1))^{1/2}\frac{|z|}{d_z}\right]\mathrm{sign}\,z,$$
$$c_{33}v\varepsilon\varphi(\mathbf{k}_1) = d_z^2\sum_{s'}{}'' V_{ss'zz}[\exp(i\mathbf{k}_1\mathbf{R}_{ss'})-1], \tag{28}$$

in the sum $\sum''$, sites s' located on the same chain as s are excluded.

Suppose, for example, that for point defects, $p_3(\mathbf{r}_1)$ is nonzero only when $\mathbf{r}_1=0$. Then according to (28), in the range $|z|\ll r_0\sim d/\varepsilon^{1/2}$ in the chain containing the defect, the strains u_{zz} have the order of magnitude $-u_0/r_0$, and the displacements $u_0 \operatorname{sign} z+u_{zz}z\approx u_0 \operatorname{sign} z$ in this range are almost constant [$u_0 \operatorname{sign} z$ is the displacement determined by formula (27)]. In neighboring chains there are displacements u_z of order u_0z/r_0, comparable with the displacements of the central chain only for $|z|\sim r_0$. When $r_1\gg d$, (28) agrees with formula (23) for u_z. These strains lead to a relatively large contribution $\sim c_{33}(u_0d)^2/r_0$ to the self-energy of the defect. This contribution might be diminished by transverse displacement of the defect (this was pointed out by A. M. Kosevich); but at sufficiently small $|u_0|\ll(dr_0)^{1/2}$, such diminution cannot compensate the increase of the energy of bending and of interaction of the chains.

We note that the characteristic features in Q1C and Q2C should carry over not only around point defects, but also near such defects as dislocations or particles of a new phase. If the dimensions of the dislocation loop or particle $R_0\ll r_0\sim d'/\varepsilon^{1/2}$, then the results presented can be applied directly at distances $r\gg R_0$. But if $R_0\gg r_0$, then a significant change of the distortion field should occur at distances $\lesssim r_0$ from the dislocation line or from the edge of a platelike (or needlelike) inclusion.

[1)] In an isolated chain, the short-range forces exerted by the defect displace, as a whole, the entire half-chain $x>d$ or $x<-d$. The forces of interaction with atoms of neighboring chains, deforming the given chain, tend to diminsh the value of the displacement. But since these forces are small, their combined action is sufficient for appreciable relative diminution of the displacement only at great distances, of the order of r_0, and only for $r\gg r_0$ do the displacement and strain fields acquire three-dimensional character.

[2)] At first glance, it seems that the large force constants $V_{ss'zz}$ for $R_{ss'}\perp Z$ should lead also to a large value of $Q^{(2)}_{\mathbf{k}zz}$. But the equilibrium conditions in the absence of stresses require fulfillment of the equality[9]

$$\sum_{s'} V_{ss'zz}R_{ss'l}R_{ss'm}=\sum_{s'} V_{ss'lm}R_{ss'z}R_{ss'z},$$

from which it is evident that with weak interaction between layers, $Q^{(2)}_{\mathbf{k}zz}$ is actually small. In the central-force model, it is easy to trace that this is a consequence of cancellation of terms $V_{ss'zz}R_{ss'l}R_{ss'm}$ with different s' in the equilibrium state. If only interaction between nearest neighbors is import, then $V_{ss'zz}=0$ and $\mu=0$; but in layered crystals, the interactions in several coordinate spheres must necessarily be significant (Ref. 10, §6).

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Translated by W. F. Brown, Jr.