

# Discrete atomic vibrations localized on defects in linear chains of atoms adsorbed by carbon nanobundles

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The conditions of the existence and the main characteristics (frequencies, intensities, and attenuation parameters) of discrete vibrational levels caused by structural defects of linear chains of inert gas atoms adsorbed on the surface of nanotubes aggregated in nanobundles, are calculated and analyzed. Discrete vibrational levels lying both above and below the band of the quasi-continuous spectrum of the chain are considered. Analytical expressions obtained for the frequencies of these discrete levels make it possible to determine with high precision the defect parameters (difference in the interaction with the substrate and with the atoms of the chain) basing on optical measurements.

Keywords: adsorbed atomic linear chains, phonon spectra, discrete localized states.

## 1. Introduction

In many cases, one-dimensional models give possibility to obtain analytical expressions for the physical quasi-particle spectra and for the physical quantities determined by these spectra. In particular, the absence of singularities within the band of a quasi-continuous spectrum of one-dimensional systems significantly simplifies the study of spectrum perturbations caused by defects. Therefore, for many years, the study of one-dimensional systems, as well as scalar models, has been used for the qualitative description of the phonon spectra and the vibrational properties of non-ideal crystal structures (see, for example, [1,2]). However, the inverse root singularities of the density of states at the edges of quasi-continuous phonon spectrum and conditioned by them instability of such structures [3] make it difficult to apply the results obtained for one-dimensional structures to real (three-dimensional) objects and, which is more important, to synthesize real one-dimensional structures. At the same time, these are the singularities that determine the non-threshold formation of discrete levels in the quasi-particle spectra caused by defects. The frequencies of discrete levels are extremely sensitive to the parameters of defects and can serve as an important source of information about the parameters of defects. Due to these properties, these chains can find direct applications, for example, in quantum computing.

The instability of one-dimensional structures (the divergence of their rms atomic displacements) is conditioned by

the inverse root singularity of the phonon densities of states at zero frequency. Placing a one-dimensional chain on any substrate eliminates the instability. A certain choice of a substrate only shifts the low-frequency singularity at the edge of the spectrum of the adsorbed chain to some non-zero frequency (see, for example, [4]) in line with a shift of an absorption edge of optical multilayers (see, for example, [5]).

The unique opportunity to create extended atomic chains is to use nanotubes (the so-called nanobundles) as substrates. The chains of atoms can be formed inside the nanotubes, in the internal channels of nanobundles, and on the surface of nanobundles in the grooves between the nanotubes. In the grooves between the nanotubes, adsorbed atoms can form linear chains of length  $\sim 10 \mu\text{m}$  or more. In the case of low concentrations of saturating gases, the one-dimensional character of objects formed by inert gases in the bundles of closed nanotubes is confirmed by studies both of neutron diffraction [6–8] and of their heat capacity [9].

Note that not all quasi-particle spectra of one-dimensional structures have inverse root singularities at the lower limit of the quasi-continuous spectrum, for example, acoustic plasmons in one-dimensional structures, formed by electrons on the surface of superfluid helium. Their spectra were obtained in [10,11].

Naturally, the adsorption of linear atomic chains on the surface of carbon nanobundles induces numerous defects in the structures of these chains. The presence of defects and the absence of a threshold for the formation of discrete vibrational levels give rise to localized states, both above and

below the band of the quasi-continuous spectrum of the chain. In [12], it was shown that even in the three-dimensional case, the characteristics of localized states can be found with high accuracy based only on the values of the first two moments of the spectral density. For the basic characteristics of localized states (their frequencies, intensities, and attenuation) simple analytical expressions can be obtained. This makes it possible to obtain localized oscillations with given frequencies, changing the parameters of defects and of the chains themselves (for example, pressure). The inversion of these formulas allows one to find the parameters of defects by experimentally measured frequencies of localized discrete levels.

We note that from the results of [12], it follows that in the linear chains the interaction between defective atoms begins to manifest itself at concentrations of defects at least by an order of magnitude higher than in three-dimensional structures. So, even at a defect concentration of more than 10%, the approximation of an isolated defect will work well.

## 2. Discrete levels localized on an isolated point defect

It is rather difficult to describe the quasi-particle spectra of systems with defects in the framework of the traditional representation of vibrations in the form of a superposition of plane waves, due to the translational symmetry of the crystal, because of the violation of translational symmetry by the defect. To avoid the difficulties one can use other methods not basing on the translational symmetry. One of these methods is the method of Jacobi matrices (J-matrices) [13–15] (see, also [11,16], where it is given in detail).

The method is based on the partition of the entire displacement space of displacements of crystal atoms into a sum of subspaces invariant with respect to the operator  $\hat{L}$  describing lattice vibrations. The vectors of the space of displacements of atoms of a crystal are the displacements of atoms along the crystallographic directions. It is convenient to choose the operator  $\hat{L}$  matrix in the form:

$$L_{ik}(\mathbf{r}, \mathbf{r}') = \frac{\Phi_{ik}(\mathbf{r}, \mathbf{r}')}{\sqrt{m(\mathbf{r})m(\mathbf{r}')}}, \text{ where } m(\mathbf{r}) \text{ is the mass of an}$$

atom with radius vector  $\mathbf{r}$ , and the matrix is  $\Phi_{ik}(\mathbf{r}, \mathbf{r}')$  the matrix of force constants, which describes the interaction between atoms with the radius vectors  $\mathbf{r}$  and  $\mathbf{r}'$ . In the operator form, the equations of the atomic vibrations of the system under consideration can be written as:

$$(\hat{L} - \varepsilon \hat{I}) \vec{\psi} = 0, \quad (1)$$

where  $\varepsilon \equiv \omega^2$  is the eigenvalue of the operator (the square of the frequency), and the wave function  $\vec{\psi}(\mathbf{r}) \equiv \sqrt{m(\mathbf{r})} \mathbf{u}(\mathbf{r})$  is the vector of space of atomic displacements  $H$ . The vectors of this space, whose dimension is  $3N$  ( $N \rightarrow \infty$  is the number of atoms in the crystal), will be denoted by the arrow above the symbol. The “ordinary” three-dimensional vectors

will be highlighted in bold (for example,  $\mathbf{u}(\mathbf{r})$  is the vector of displacement of an atom with the radius vector  $\mathbf{r}$  from the equilibrium position).

If in the space of atomic displacements we choose some vector  $\vec{h}_0 \in H$  (call this vector generating), then the linear span of the set of vectors  $\{\hat{L}^n \vec{h}_0\}_{n=0}^{\infty}$  is a subspace of the space  $H$  invariant with respect to the operator  $\hat{L}$ . By orthonormalization of the sequence  $\{\hat{L}^n \vec{h}_0\}_{n=0}^{\infty}$ , we obtain the  $\{\vec{h}_0\}_{n=0}^{\infty}$  basis. In this basis, the operator generated by the operator  $\hat{L}$  in the corresponding invariant subspace is represented by the three-diagonal (Jacoby) matrix:

$$L_{ik} = a_i \delta_{ik} + b_i (\delta_{i,k+1} + \delta_{i+1,k}). \quad (2)$$

Matrix elements (2) have a remarkable property. If the band of the quasi-continuous spectrum of the operator  $\hat{L}$  is simply connected, then with growth of  $n$  they tend to some limiting values:

$$\lim_{n \rightarrow \infty} a_n = a, \quad \lim_{n \rightarrow \infty} b_n = b, \quad (3)$$

and  $a$  is the value of the middle of the band of the continuous spectrum, and  $b$  is a quarter of the width of this band.

Often matrix elements (2) tend to limit values very fast, and for linear chains only the first one or two elements differ from the values (3). Therefore, to solve our problem, we consider the spectrum of the J-matrix  $L_{ik} = a \delta_{ik} + b(\delta_{i,k+1} + \delta_{i+1,k})$  first. If the operator  $\hat{L}$  is represented as a Jacobian matrix, then the element  $G_{00}(\varepsilon)$  of the operator  $\hat{G}(\varepsilon) \equiv (\hat{L} - \varepsilon \hat{I})^{-1}$  (the so-called Green operator of Eq. (1)) is represented as a continued fraction. For the J-matrix, the fraction  $L_{ik}^{(\infty)} = a \delta_{ik} + b(\delta_{i,k+1} + \delta_{i+1,k})$  has the form:

$$G_{00}(\varepsilon) \equiv (\hat{L} - \varepsilon \hat{I})_{00}^{-1} = 2b^{-2} \left[ \varepsilon - a + Z(\varepsilon) \sqrt{|\varepsilon - (a - 2|b|)| |\varepsilon - (a + 2|b|)|} \right], \quad (4)$$

where, the function  $Z(\varepsilon)$  determines the difference in the behavior of the Green function in the band of the quasi-continuous spectrum and beyond it

$$Z(\varepsilon) \equiv \Theta(-\varepsilon + a - 2|b|) + i \Theta(\varepsilon - a + 2|b|) \times \Theta(-\varepsilon + a + 2|b|) - \Theta(\varepsilon - a - 2|b|). \quad (5)$$

In (5),  $\Theta(x)$  is the Heaviside theta function.

Thus,  $\mathcal{D}$ , that is the band of the quasi-continuous spectrum of the operator  $\hat{L}$ , is the interval  $\varepsilon \in [a - 2|b|, a + 2|b|]$ . The real and imaginary parts of the function (4) are presented in Fig. 1.

If localized discrete levels arise outside the  $\mathcal{D}$  band under the influence of some perturbation, then these levels are the roots of the Lifshitz equation (see, for example, [1]). This equation can be written as:

$$G_{00}(\varepsilon) = S(\varepsilon, \{\Lambda_s\}). \quad (6)$$

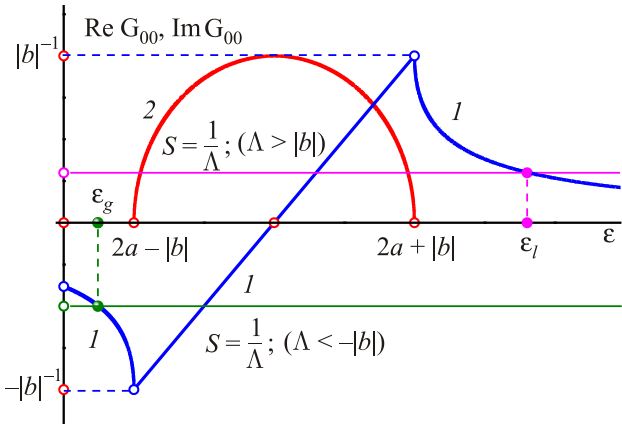


Fig. 1. The real (curve 1) and imaginary (curve 2) parts of the Green function (4), and the solution of Eq. (6) for the case of a first-rank perturbation operator.

The perturbation operator is denoted by  $\hat{\Lambda}$ . Recall that for  $\epsilon \notin \mathcal{D}$ , the function (4) is real. The function  $S(\epsilon, \{\Lambda_s\})$  is determined by the operator  $\hat{\Lambda}$  and depends on the set of parameters  $\{\Lambda_s\}$  characterizing this operator. For the case, when the J-matrix of the perturbed operator  $\hat{L} + \hat{\Lambda}$  differs from the matrix  $L_{ik}^{(\infty)}$  only by the value of its first diagonal element  $a_0 = a + \Lambda$ , the function  $S(\epsilon, \{\Lambda_s\})$  becomes the constant  $S \equiv \Lambda^{-1} = \text{const}$ . Note that it is the form peculiar for perturbation operators describing defects in an adsorbed linear chain that correspond to a local change in the atomic bond with the substrate or a local change in one bond between the atoms of the chain [17,18]. In this case, from Fig. 1, it is seen that localized states with squares of frequency  $\epsilon_g < a - 2|b|$  appear at perturbation values  $\Lambda < -|b|$ , and localized states with squares of frequency  $\epsilon_l > a + 2|b|$  appear at  $\Lambda > |b|$ .

The Green function of the perturbed operator  $\tilde{G}_{00}(\epsilon, \Lambda) \equiv (\hat{L} + \hat{\Lambda} - \hat{I}\epsilon)_{00}^{-1}$  can be represented as

$$\tilde{G}_{00}(\epsilon, \Lambda) = \frac{1}{\epsilon - a - \Lambda - b^2 G_{00}(\epsilon)}, \quad (7)$$

where, the function  $G_{00}$  is determined by the relation (4). The function (7) is easy to transform to:

$$\tilde{G}_{00}(\epsilon, \Lambda) = -\frac{1}{2} \frac{\epsilon - a - 2\Lambda + Z(\epsilon) \sqrt{(\epsilon - a)^2 - 4b^2}}{\Lambda(\epsilon - a) - (\Lambda^2 + b^2)}. \quad (8)$$

The pole of this function defines the square of the frequency of the discrete level

$$\epsilon_d = a + \frac{\Lambda^2 + b^2}{\Lambda}, \quad (9)$$

at  $\Lambda > |b|$  the value  $\epsilon_d \equiv \epsilon_l > a + 2|b|$ ,  
 at  $\Lambda < -|b|$  the value  $\epsilon_d \equiv \epsilon_g < a - 2|b|$ .

The residue of the function (8) at the pole (9) determines the intensity of a given level — the relative amplitude of oscillations of the atoms of the defect at frequency  $\sqrt{\epsilon_d}$ .

$$\mu_0(\epsilon_d, \Lambda) = \text{re}'s_{\epsilon=\epsilon_d} \tilde{G}_{00}(\epsilon) = \frac{1}{2\Lambda} \left[ \frac{\Lambda^2 - b^2}{\Lambda} - Z(\epsilon) \left| \frac{\Lambda^2 - b^2}{\Lambda} \right| \right]. \quad (10)$$

The value (10) is nonzero only when the conditions for the existence of discrete levels are fulfilled. For  $\epsilon_d \equiv \epsilon_g < a - 2|b|$ , when  $Z(\epsilon) = 1$ , this condition is  $\Lambda < -|b|$ , and for  $\epsilon_d \equiv \epsilon_l > a + 2|b|$ , when  $Z(\epsilon) = -1$ , this condition is  $\Lambda > |b|$ . In both cases, the intensity of the discrete level is equal to:

$$\mu_0(\epsilon_d, \Lambda) = \frac{\Lambda^2 - b^2}{\Lambda^2}. \quad (11)$$

The damping of the amplitude of oscillations at the given level is characterized by a decrease of the values  $\mu_n(\epsilon_d, \Lambda) = \text{re}'s_{\epsilon=\epsilon_d} \tilde{G}_{nn}(\epsilon)$  when  $n$  increase. Using the relations obtained in [12], it can be shown that the quantities  $\mu_n(\epsilon_d, \Lambda)$  form an infinite decreasing geometric progression  $\mu_n(\epsilon_d, \Lambda) = \mu_0(\epsilon_d, \Lambda) \left(\frac{b}{\Lambda}\right)^{2n}$ , the sum of which is equal to the unit, that is, one quasi-particle splits off from a continuous spectrum band to a discrete level.

### 3. Discrete localized vibrations in adsorbed linear chains

Recently, adsorption of inert gas atoms onto bundles of carbon nanotubes has often been used to obtain stable macroscopically long quasi-one-dimensional objects [4,6–8,19–22]. In the case of a low concentration of adsorbed gases, their atoms are located in the grooves between the nanotubes on the surface of the nanobundle (and in the case of  $^4\text{He}$ , inside nanobundles and even nanotubes). In the grooves between the nanotubes, adsorbed atoms can form linear chains with a length of  $\sim 10 \mu\text{m}$ . The length corresponds to the number of atoms in the chain  $\sim 10^3 - 10^4$ , and thus the boundary effects can be neglected. The one-dimensional nature of these objects is confirmed by both neutron diffraction studies [6–8] and experiments on measurements of heat capacity [9,19–22].

Neutron diffraction studies of  $^4\text{He}$  atoms adsorbed in the grooves on the surface of nanobundles showed the periodicity of the arrangement of atoms in the chain [6], and theoretical calculations [23] showed the presence of a periodic potential along the grooves on the surface of nanobundles. The depth of this potential varies from the values insignificantly greater than zero to 40 K and depends on the relative orientation and displacement of the nanotubes forming the groove. All this makes it possible to describe the vibrational characteristics of the chains adsorbed in the

grooves between the nanotubes within the framework of the harmonic dynamics of the crystal lattice.

In [4], it was shown that, starting from a certain frequency, the vibrations of the atoms of the chain in the groove between the nanotubes are either quasi-localized or have a one-dimensional character. The previously mentioned initial frequency is determined by the contribution of the interaction of the atoms of the chain with the atoms of the nanotube to the self-interaction matrix of the chain. Also in [4] it was shown that a chain of atoms adsorbed in a groove between nanotubes with a sufficiently high degree of accuracy can be considered as a chain in an external field that determines the initial frequency of its quasi-continuous spectrum. The width of this spectrum is determined by the interaction of atoms in the chain with each other, which in turn depends on the distance  $r$  between them. In this approximation, the problem of the vibrational spectrum of the adsorbed chain without defects is reduced to two parameters: the minimum and maximum frequencies of its quasi-continuous spectrum [4]. This approximation can be successfully applied to the chains of inert gas atoms adsorbed on a carbon substrate due to the large difference between the Debye temperatures of inert gases and carbon structures.

Because of the interaction of the atoms of the adsorbed chain with the atoms of carbon nanotubes, the distance between the atoms of the chain does not coincide with the equilibrium distance  $r_0$  corresponding to the minimum of the potential of interatomic interaction of the adsorbed atoms. In the case  $r < r_0$  (see, for example, [7]) the non-central interaction parameter, which determines the width of the spectrum of transverse vibrations, is negative. It leads to a shift of the minimum frequency of the quasi-continuous spectrum to the region of low frequencies [17,18]. A compressed chain can be formed by inert gas atoms ( $r < r_0$ ) due to the fact that the period of the field created by nanotubes in the grooves is less than the equilibrium distance for all inert gases except helium [23]. The negative value of the non-central interaction parameter is inherent in many solidified gases and metals [7,21–23].

The operator describing interatomic interactions in the coordinate representation can be written in the form:

$$L_{ik}(\mathbf{r}, \mathbf{r}') = \frac{(\varepsilon_{l0} + 2\alpha)\delta_{\mathbf{r}, \mathbf{r}'} - \alpha(\delta_{\mathbf{r}, \mathbf{r}'+a} + \delta_{\mathbf{r}, \mathbf{r}'-a})}{m} \delta_{ix} \delta_{ik} + \frac{(\varepsilon_{\tau 0} + 2\beta)\delta_{\mathbf{r}, \mathbf{r}'} - \beta(\delta_{\mathbf{r}, \mathbf{r}'+a} + \delta_{\mathbf{r}, \mathbf{r}'-a})}{m} (\delta_{iy} + \delta_{iz}) \delta_{ik}, \quad (12)$$

where  $a$  is the interatomic distance in the chain,  $m$  is the mass of the atom, the parameters  $\alpha$  and  $\beta$  describe, respectively, the central and non-central interaction between the atoms. For a pair-wise isotropic interaction between atoms, these parameters are expressed in terms of the potential of this interaction  $\varphi(r)$  as follows:

$$\alpha(r) = \frac{\partial^2 \varphi(r)}{\partial r^2}; \quad \beta(r) = \frac{1}{r} \frac{\partial \varphi(r)}{\partial r}.$$

The dispersion relations arising from (1) in this case have the form:

$$\begin{aligned} \varepsilon_l(k) &\equiv \omega_l^2(k) = \varepsilon_{0l} + \frac{4\alpha}{m} \sin^2 \frac{ka}{2}, \\ \varepsilon_\tau(k) &\equiv \omega_\tau^2(k) = \varepsilon_{0\tau} + \frac{4\beta}{m} \sin^2 \frac{ka}{2}. \end{aligned} \quad (13)$$

Here  $k$  is the quasi-wave vector, the subscripts  $l$  and  $\tau$  denote the longitudinally and transversely polarized vibrational modes, respectively. Note that the symmetry condition of the tensor of elastic modules should be applied to the whole system (including not only the chain, but also the substrate), since it is the interaction of the chain with the substrate that ensures its stability. Therefore, the transverse vibrations of the atoms of the chain (13) are not flexural with the dispersion  $\varepsilon_\tau(k) \sim k^4$  in the long-wavelength region (see, for example, [1]).

The defects of nanotubes, as well as the incommensurability of the periods of the adsorbed chain and the field in the groove between the nanotubes, can lead to a local change in the interaction of the atoms of the chain with the nanotubes. In the case of a local change in the interaction, the distance between pairs of atoms of the chain can also change, which, in turn, can lead to the appearance of localized states with frequencies both below the minimum frequency of the quasi-continuous spectrum of the chain and above its maximum frequency.

For solving the problem of the vibrational characteristics of the chain with such a defect using the Jacoby matrix method, the space of displacements of the chain atoms  $H$  should be represented for each direction  $i$  as a direct sum of subspaces orthogonal to each other:  $H = \sum_i (H_i^{(-)} \oplus H_i^{(+)})$ . The subspaces  $H_i^{(-)}$  are the subspaces of in-phase displacements of atoms, and the subspaces  $H_i^{(+)}$  are the subspaces of anti-phase displacements. For each of the directions of atomic displacements, these subspaces are linear spans of the set of vectors  $\{\hat{L}^n \vec{h}_0^{(-)}\}_{n=0}^\infty$  and  $\{\hat{L}^n \vec{h}_0^{(+)}\}_{n=0}^\infty$ , respectively (further the index  $i$  will be omitted, except when the direction of displacement is significant). The generating vectors  $\vec{h}_0^{(-)} = \frac{1}{\sqrt{2}} \begin{vmatrix} -a/2 & 1 \\ a/2 & 1 \end{vmatrix}$  and  $\vec{h}_0^{(+)} = \frac{1}{\sqrt{2}} \begin{vmatrix} -a/2 & 1 \\ a/2 & -1 \end{vmatrix}$  correspond to the in-phase and anti-phase displacements of two neighboring atoms (the origin of coordinates is chosen at the center of symmetry of the defect).

The matrix elements of the Jacoby matrices of the operators  $\hat{L}^{(-)}$  and  $\hat{L}^{(+)}$ , induced by the operator  $\hat{L}$  in each of the corresponding subspaces, differ from (3) only by the values of the first diagonal elements  $a_0$



$$\begin{aligned} a_0^{(-)} &= a - b + \varepsilon_0 \delta, \\ a_0^{(+)} &= a + b + \varepsilon_0 \delta + 2b\eta, \end{aligned} \tag{14}$$

where  $\varepsilon_0 \equiv a - 2b$  is the value of the square of the frequency at  $k = 0$ , that is, the activation frequency for an ideal atom,  $\varepsilon_0(1 + \delta)$  is the activation frequency for the defective atom; the parameter  $\eta$  characterizes the change caused by the defect in the corresponding force constant ( $\alpha$  for the longitudinal displacements and  $\beta$  for the transverse ones, further to be distinguished as  $\eta_l$  and  $\eta_\tau$ ). That is, for the operators describing the perturbation induced by the defect, we obtain

$$\begin{aligned} \Lambda_l^{(-)} &= -\alpha + \varepsilon_0 \delta, & \Lambda_\tau^{(-)} &= -\beta + \varepsilon_0 \delta, \\ \Lambda_l^{(+)} &= \varepsilon_0 \delta + \alpha(1 + 2\eta), & \Lambda_\tau^{(+)} &= \varepsilon_0 \delta + \beta(1 + 2\eta). \end{aligned} \tag{15}$$

In (15), for longitudinal displacements the matrix element  $b = \alpha$ , and for transverse ones  $b = \beta$ . We emphasize again that the parameter  $\alpha$  is always positive, and the parameter  $\beta$  can take negative values [7,17,24,25]. Then for any direction we can write:

$$\Lambda^{(-)} = -b + \varepsilon_0 \delta; \quad \Lambda^{(+)} = \varepsilon_0 \delta + b(1 + 2\eta). \tag{16}$$

The conditions of occurrence of discrete levels with frequencies above the quasi-continuous spectrum band are: in the subspaces  $H_i^{(-)}$

$$\begin{aligned} \varepsilon_0 \delta > 2b, & \text{ for } b > 0; \\ \delta > 0, & \text{ for } b < 0; \end{aligned} \tag{17}$$

in the subspaces  $H_i^{(+)}$

$$\begin{aligned} \varepsilon_0 \delta + 2b\eta > 0, & \text{ for } b > 0; \\ \varepsilon_0 \delta - 2|b|\eta > 2|b|, & \text{ for } b < 0. \end{aligned} \tag{18}$$

The conditions of occurrence of discrete levels with frequencies below the quasi-continuous spectrum band are: in the subspaces  $H_i^{(-)}$

$$\begin{aligned} \delta < 0, & \text{ for } b > 0; \\ \varepsilon_0 \delta < -2|b|, & \text{ for } b < 0; \end{aligned} \tag{19}$$

in the subspaces  $H_i^{(+)}$

$$\begin{aligned} \varepsilon_0 \delta + 2b\eta < -2b; & \text{ for } b > 0; \\ \varepsilon_0 \delta - 2|b|\eta < 0; & \text{ for } b < 0; \end{aligned} \tag{20}$$

(the index  $i$  can be omitted).

From (9) and (16), for the values  $\varepsilon_d^{(-)}$  and  $\varepsilon_d^{(+)}$  of the localized discrete levels in the invariant subspaces  $H^{(-)}$  and  $H^{(+)}$ , we obtain:

$$\begin{aligned} \varepsilon_d^{(-)} &= \varepsilon_0 + \frac{\varepsilon_0^2 \delta^2}{\varepsilon_0 \delta - b}, \\ \varepsilon_d^{(+)} &= \varepsilon_0 + \frac{[\varepsilon_0 \delta + 2b(1 + \eta)]^2}{\varepsilon_0 \delta + b(1 + 2\eta)}. \end{aligned} \tag{21}$$

Whether this level is formed above or below the band of a quasi-continuous spectrum is determined by the relations (17), (20). Having solved the system (21) with respect to the parameters of the defect  $\delta$ , and  $\eta$  we obtain the expressions for these quantities via experimentally measured frequencies of the localized discrete levels:

$$\begin{aligned} \delta &= \varepsilon_0^{-1} \cdot \left[ \frac{\varepsilon_0^{(-)} - \varepsilon_0}{2} - b \pm \sqrt{\frac{\varepsilon_0^{(-)} - \varepsilon_0}{2} \cdot \left( \frac{\varepsilon_0^{(-)} - \varepsilon_0}{2} - 2b \right)} \right], \\ \eta &= \frac{1}{2b} \cdot \left[ \frac{\varepsilon_0^{(+)} - \varepsilon_0}{2} - b \pm \sqrt{\frac{\varepsilon_0^{(+)} - \varepsilon_0}{2} \cdot \left( \frac{\varepsilon_0^{(+)} - \varepsilon_0}{2} - 2b \right)} - \varepsilon_0 \delta \right], \end{aligned} \tag{22}$$

(the “+” sign in front of the radical corresponds to the discrete localized level lying above the band of the quasi-continuous spectrum, and the sign “-” corresponds to the discrete localized level lying below the band). Atomic displacement vectors related to the subspaces  $H_i^{(-)}$  and  $H_i^{(+)}$  are transformed according to different irreducible representations of the symmetry group of the chain, which consists of one element that is inversion: even (subspace) and odd (subspace).

Atomic displacement vectors related to subspaces  $H_i^{(-)}$  and  $H_i^{(+)}$  are transformed according to different irreducible representations of the symmetry group of the chain, odd and even, respectively. Therefore, the localized discrete levels in the subspaces  $H_i^{(+)}$  are Raman active, and in the subspaces  $H_i^{(-)}$ , are infrared active.

#### 4. Conclusion

Thus, we have shown that defects such as local changes in the distances between atoms in the linear chains adsorbed on the surface of carbon nanobundles often form localized states in the phonon spectrum of the chains with frequencies both above and below the quasi-continuous band. Such states arise in a wide range of defect parameters (changes in the interaction with the substrate and changes in the interaction between the atoms of the defect). Measuring the frequencies of such localized states, for example, in experiments on Raman (see, for example, [26]), or infrared (see, for example, [5]) light scattering, makes it possible to determine these defect parameters using the simple analytical expressions obtained in this work.

Note that the results of this work were obtained for an isolated defect, but for the linear chains this approximation, is applicable for concentrations of these defects above 10%, unlike three-dimensional structures, where this approximation ceases to be applicable even at much smaller (~2%) concentrations defect [27,28]). Naturally, in the adsorbed chains, several similar defects may emerge, which will form several localized discrete levels. The frequencies of each of these levels can be measured (in particular, by optical methods), and the parameters of each defect can determined from their frequencies.

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Локалізовані на дефектах дискретні коливальні рівні в лінійних ланцюжках атомів, адсорбованих вуглецевим нанобандлом

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Розраховано та проаналізовано умови існування та основні характеристики (частоти, інтенсивності та параметри згасання) дискретних коливальних рівнів, які обумовлені дефектами структури лінійних ланцюжків атомів інертних газів, адсорбованих на поверхню зв'язаних в нанобандл нанотрубок. Розглянуто дискретні коливальні рівні, що лежать як вище, так і нижче смуги квазібезперервного спектру ланцюжка. Одержані для частот цих дискретних рівнів аналітичні вирази дозволяють надійно знаходити параметри дефекту (відмінність його взаємодії з підкладкою та атомами ланцюжка) за результатами оптичних вимірювань.

Ключові слова: адсорбовані атомні лінійні ланцюжки, фононні спектри, дискретні локалізовані стани.

Локализованные на дефектах дискретные колебательные уровни в линейных цепочках атомов, адсорбированных углеродным нанобандлом

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Рассчитаны и проанализированы условия существования и основные характеристики (частоты, интенсивности и параметры затухания) дискретных колебательных уровней, которые обусловлены дефектами структуры линейных цепочек атомов инертных газов, адсорбированных на поверхность связанных в нанобандл нанотрубок. Рассмотрены дискретные колебательные уровни, лежащие как выше, так и ниже полосы квази-непрерывного спектра цепочки. Полученные для частот данных дискретных уровней аналитические выражения позволяют надежно определять параметры дефекта (отличие его взаимодействия с подложкой и атомами цепочки) по результатам оптических измерений.

Ключевые слова: адсорбированные атомные линейные цепочки, фононные спектры, дискретные локализованные состояния.