The Influence of a Point Impurity on the Phonon Spectrum of a Chain of Noble Gas Atoms Adsorbed on a Carbon Nanobundle.

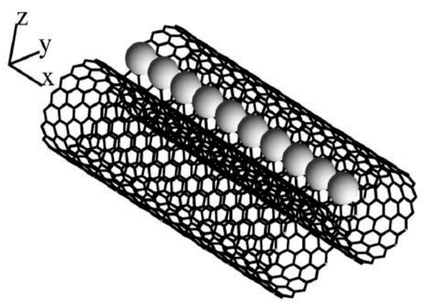
E.V. Manzhelii[1], S.B. Feodosyev[1], E.S. Syrkin[1]

B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine
47 Nauky Ave., Kharkiv, 61103, Ukraine
emanzhelii@ilt.kharkov.ua

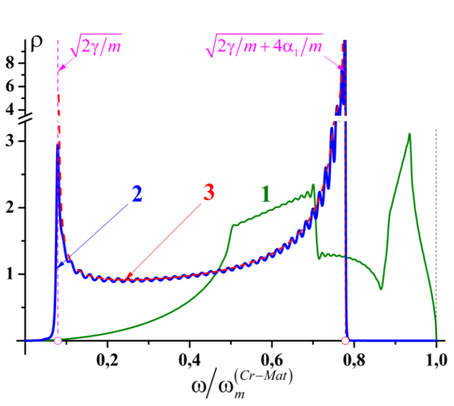
The synthesis and experimental study of long chains of inert gas atoms adsorbed in grooves on the surface of carbon nanotube bundle aroused interest in the theoretical study of the vibrational and thermodynamic properties of these chains.The linear and periodic nature of these objects is directly confirmed by neutron diffraction studies. The linear and periodic nature of these chains is indirectly confirmed by studying their low-temperature heat capacity .

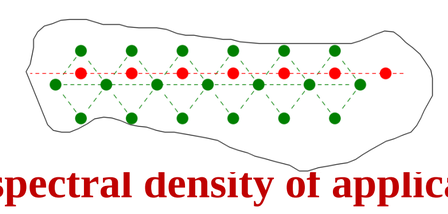
The stability of the adsorbed chains of atoms is determined by the interaction of the atoms of the chain with the substrate. As a result of this interaction, the spectrum of the adsorbed chain starts with a nonzero frequency. Localized vibrations generated by a substitution impurity can occur both below the initial frequency and above the maximum frequency of the quasi-continuous spectrum of the chain. We considered a point impurity that differs from the atoms of the chain in mass, in interaction with the atoms of the chain, and in the interaction with the substrate. We consider a chain of adsorbed atoms as a chain in a periodic external field. In this approximation, we obtained analytical expressions for the oscillation frequencies as functions of these three parameters. Analytical expressions for the thresholds for the occurrence of localized oscillations and the intensity of localized oscillations were also obtained. These results make it possible to further theoretically study in the effect of point impurities on the low-temperature heat capacity of chains of inert gas atoms adsorbed in grooves on the surface of carbon nanobundles.

DEFECT- FREE LEAR CHAIN

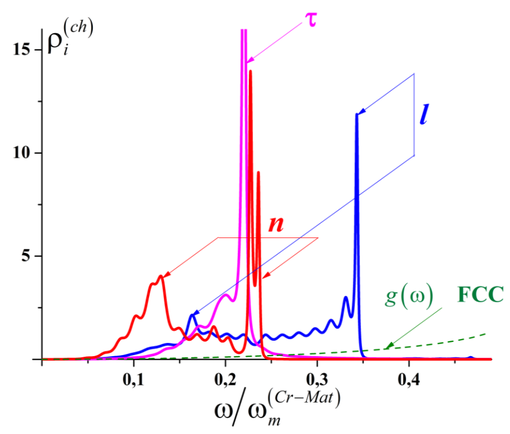


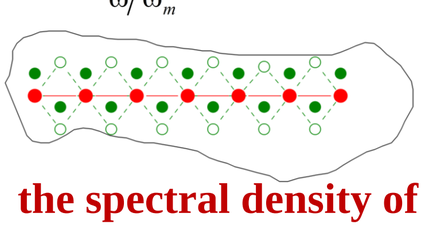
one – dimensional atomic structure adsorbed by a carbon nanotube bundle



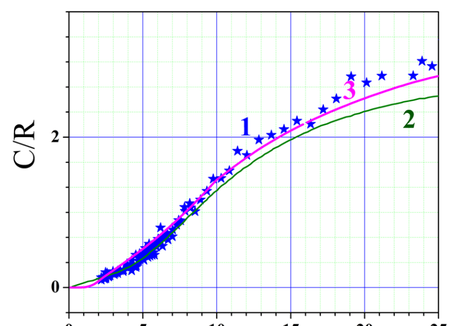


the spectral density of applicated chain





the spectral density of the embedded chain



the heat capacity

POINT IMPURITY

$m_d = m(1+\varepsilon)$ **change in the external field**

$f_d = f(1+\xi)$ **change in the mass of the atom**

$\alpha_{id} = \alpha_i(1+\eta_i),\ i = l, \tau$ **change in the interaction between the atoms of the chain**

LOCALIZED OSCILATIONS IN THE SUBSPACE OF ANTIPHASE DISPLACEMENTS

$$\lambda_{di}^{(-)} = \frac{b_i^2 + \left(\Lambda_{00i}^{(-)}\right)^2}{\Lambda_{00i}^{(-)}} + a_i;$$

$$a_i = \frac{2\alpha_i + f}{m};\quad b_i = \frac{\alpha_i}{m};\quad \Lambda_{00i}^{(-)} = \frac{\eta_i \alpha_i}{m};$$

energy of the levels

$$\lambda_{di}^{(-)} < \lambda_{\min i} \qquad \Lambda_{00i}^{(-)} < -|b_i|$$

$$\lambda_{di}^{(-)} > \lambda_{\max i} \qquad \Lambda_{00i}^{(-)} > |b_i|$$

threshold

LOCALIZED OSCILATIONS IN THE SUBSPACE OF INPHASE DISPLACEMENTS

$$\lambda_{di}^{(0)} = \frac{-B_i \pm \sqrt{B_i^2 - 4A_iC_i}}{2A_i}$$

$$B_i = 2\left[\left(1-\gamma_i^2\right)\left(\tilde{a}_{0i}^{(+)} + \gamma_i^2 a\right) + 2\gamma_i^4 a_i\right]$$

$$C_i = \left(a_{0i}^{(+)} + \gamma_i^2 a\right)^2 - \gamma_i^4 \lambda_{\min i}\lambda_{\max i}$$

$$\gamma_i = \frac{1+\eta_i}{\sqrt{1+\varepsilon}}$$

$$\tilde{a}_{0i}^{(0)} = \frac{2\alpha_i(1+\eta_i)}{m(1+\varepsilon)} + \frac{f_i(1+\xi_i)}{m(1+\varepsilon)}$$

energy of the levels

$A_i = 1 - 2\gamma_i^2$

Localized vibrations are formed without a threshold.

In every subspace one phonon splits off from the quasi-continuous spectrum band to the discrete level.