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Phonon spectrum and vibrational characteristics of l inear nanostructures in solid m atrices

Nowadays, the structures with one-dimensional or quasi-one-dimensional nanoinclusions in various crystalline or amorphous matrices attract attention of researchers. Under real relations between the interactions of the atoms of embedded quasi-periodic systems with each other and with the atoms of the matrix, the features, inherent to one-dimensional systems, can appear in the quasi-particle spectra of these structures.

Key words: Matrix nanostructure crystal structure of amorphous.

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Фононный спектр и колебательные характеристики линейных наноструктур в твердых матрицах

В настоящее время структуры с одномерным или квази-одномерным включением в различных кристаллических или аморфных матрицах привлекают внимание исследователей. В реальных отношениях между взаимодействиями атомов встроенных квазипериодических систем друг с другом и с атомами матрицы особенности, присущие одномерным системам, могу появиться в спектрах квазичастиц этих структур.

Ключевые слова: матрица, наноструктуры, кристалл, аморфная структура.

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Қатты матрицалардағы сызықты наноқұрылымдардың тербеліс сипаттамалары және фононды спектр

Қазіргі уақытта әртүрлі кристалл немесе аморфты матрицаларға бірөлшемді немесе квазибірөлшемді қосылған құрылымдар зерттеушілердің назарын аударып отыр. Кіріктірілген квазипериодты жүйелердің атомдарының бір-бірімен және матрица атомдарымен өзара әрекеттесуінің шынайы қатынастарында бірөлшемді жүйелерге тән ерекшеліктер осы құрылымдардың квазибөлшектерінің спектрлерінде пайда болуы мүмкін.

Түйін сөздер: матрица, наноқұрылымдар, кристалл, аморфты құрылым.

Nowadays, the structures with one-dimensional or quasi-one-dimensional nanoinclusions in various crystalline or amorphous matrices attract attention of researchers. Under real relations between the interactions of the atoms of embedded quasi-periodic systems with each other and with the atoms of the matrix, the features, inherent to one-dimensional systems, can appear in the quasi-particle spectra of these structures. The one-dimensional chains are known to be unstable (e.g. [1]) and such a behavior of the phonon spectrum can significantly reduce the dynamic stability of the system, namely, enlarge the root-mean-square (rms) amplitudes of atomic displacements. Therefore, the existing of quasi-one-dimensional features in the systems with high stability seems to be important and interesting problem.

In the present paper, the atomic dynamics of linear chains embedded in a crystalline matrix or adsorbed on its surface is studied. A linear chain

formed by substitutional impurities in a surface layer and at the same time offsetting from this layer was analyzed particularly. This system models the actively studied experimentally structures in which gas molecules (monatomic or diatomic) are adsorbed on the walls of the bundles of carbon nanotubes located in certain medium [2].

It is shown that the quasi-1D features are typical for the chains in which the interatomic interaction is 2÷3 times higher than the interaction between the atoms of the chain and the atoms of the crystal matrix. On the local phonon density of atoms of the chain, the transition to quasi-one-dimensional behavior has the form of the kink. In other words, it is the first (lowest-frequency) van Hove singularity, which in 3D structures (the system under consideration is generally three-dimensional) corresponds to the transition from closed to open constant-frequency (quasi-plane) surfaces. The local phonon densities of atoms in the chain have one-dimensional character at frequencies higher than the frequency of the van Hove singularity. The rms-amplitude of embedded chains atoms vibrations is calculated and the behavior of the atomic vibrations contribution in the low-temperature heat capacity of the system is analyzed. The influence of substitutional impurities in quasi-one-dimensional nano-inclusions on their phonon spectra was studied, in particular, the conditions of forming and the characteristics of the localized states in both the high-frequency and low-frequency regions of the phonon spectrum of the system.

Analytical expressions for the phonon spectral densities of the atoms of linear chains with defects in periodic external field are obtained.

References

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