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AN EXAMPLE OF IMPURITY-INDUCED LOCAL VIBRATIONS IN CLUSTERS

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ПРОСТОЙ ПРИМЕР ИНДУЦИРОВАННОГО ПРИМЕСЬЮ ЛОКАЛЬНОГО КОЛЕБАНИЯ В КЛАСТЕРАХ. Николай КРИСТОФЕЛЬ

Key words: atomic clusters, local modes.

Investigation of various properties of atomic clusters is a rapidly developing field in condensed matter physics at present. Further stimulation here stems from the discovery of fullerene and its derivatives. Atomic clusters of interest may consist of a large number of atoms. There may be nonregular atoms, which are considered as impurities (defects) and, analogously to crystals, the problem of induced localized states arises for clusters from both experimental and theoretical point of view. For crystals this problem has been widely investigated and solved. For clusters it seems to have only just started.

Concerning the problem mentioned in the framework of atomic cage dynamics, a simple example including clusters is presented here basing on the results of paper [1]. There the frequencies of even localized modes generated in a chain of $N + 1$ atoms (N-even) by a defect changing the force constants with nearest neighbours, has been found. The equations of motion are of the form

$$\frac{m\partial^2 q_1}{k\partial t^2} = q_2 - (1+P)\, q_1, \tag{1}$$

$$\frac{m\partial^2 q_n}{k\partial t^2} = q_{n+1} + q_{n-1} - 2q_n \qquad \left(n \neq 0,\ 1,\ \frac{N}{2}\right).$$

Here $P = \frac{\Upsilon}{k}$ is the relation of perturbed force constant to unperturbed one.

The localized mode frequencies are given by

$$\omega_l^2 = \frac{2k}{m}(1 + ch\kappa), \tag{2}$$

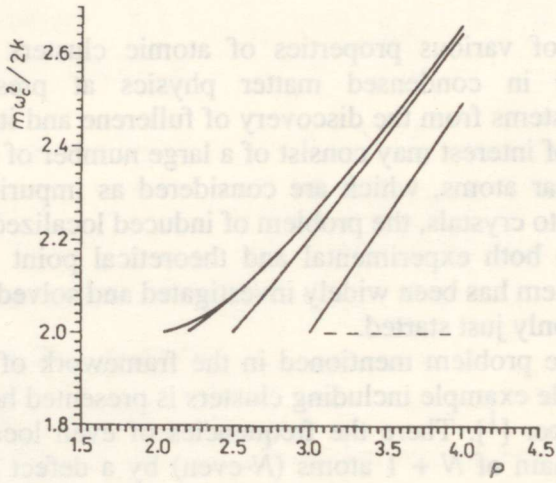
where κ is determined by the equation, which corresponds to the fixed end boundary condition

$$sh\frac{N\kappa}{2} = (P-1)\, sh\left(\frac{N}{2} - 1\right)\kappa. \tag{3}$$

The upper vibration band edge of the unperturbed system equals $\omega_m^2 = \frac{4k}{m}$. For $ch\kappa > 1$, $\omega_l > \omega_m$ and the nature of the corresponding mode is such that atomic shifts decrease moving away from the impurity:

$$q_n(l) = A_l e^{i\omega_l t}\,[shn\kappa + (1-P)\, sh\,(n-1)\,\kappa] \tag{4}$$

for $n > 0$, $q_n = -q_{-n}$. It means that also in clusters (moderate N) there may be localized vibrations present in the same sense as for crystals. However, it must be stressed that not a free cluster has been considered here, the fixed end boundary conditions acting for a build-up of a "crystalline" unperturbed band.



Dependence of the local mode frequency on the perturbation parameter.

To create such a mode the perturbation must exceed the N-dependent critical value

$$P_k = \frac{N-1}{0.5N-1}. \tag{5}$$

For an infinite crystal $N \to \infty$, $P_k = 2$. As P_k rises with the diminishing of N, the creation of localized vibrations in clusters requires a stronger perturbation. The situation is reflected by the curves $\omega_i^2(P)$ in Figure for $N = 4; 6; 12; 50$ from the right. The unperturbed band edge is shown by the broken line. The difference between the "cluster" and the "crystal" practically disappears between $N = 12$ and 50. One must keep in mind that the form of the cluster is considered independent of the number of atoms in it. In real non-onedimensional cases it need not be so.

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