LATTICE PARAMETERS MODIFICATION OF PARA-DICHLORBENZOL NANODIMENSION FILMS

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Influence of decrease of the sizes of crystallites of para-dichlorbenzol on Raman spectrums is studied. Lattice oscillations frequencies are calculated. On this basis the modification of lattice parameters for particles smaller than 5μ and an incremented modification of nanodimension sized particles are studied. Magnification of lines intensities are related to transmitting oscillations and orientation oscillations frequency decrease is found.

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As it is scored in a number of operations of a lattice of [1] parameters nanodimension particles constructed on atoms differ from parameters of a lattice of crystals of the greater size. Thus for one crystal the sizes of a lattice can be incremented, for others will decrease. The modification of physical properties because of resizing crystallites for the structures constructed of organic molecules, apparently, should be observed at their greater size, than for the structures constructed of atoms. Organic crystallites find the increasing application in the molecular electronics engineering (at making crystals, and in units of storage). Therefore as will lead parameters of a lattice for organic molecular crystals at decrease of particle sizes up to nanodimensions, represents practical interest. For learning this problem it has been carried out examination of particles from 5μ and below ~1μ organic matter by a method of a Raman effect of light of small frequencies. This method has been selected, as spectrums of the lattice oscillations are rather sensitive to modify structure of a crystal. As the object of examination the molecular crystal of para-dichlorbenzol which is the good modelling object has been selected. Para-dichlorbenzol was studied by various methods. It crystallizes in space group P2₁/a with two molecules in cell [2].

Samples were prepared by a following method. On a glass plate (an integumentary glass) the studied crystal has been raised out of dust. A film derived consist, apparently, from separate crystallites. After a sputtering the film was evaporated up to the necessary width. It has been prepared three exemplars by width from 30μ, ~5μ and less 1μ. The film consists of separate crystallites. From above the received film of the necessary width has been covered by other integumentary glass, for decrease of transpiration. After that Raman spectrums of small frequencies have been received.

In Fig. 1 the spectrums of the lattice oscillations obtained for films of studied width of para-dichlorbenzol are shown. In a spectrum of the lattice oscillations of a single crystal it should be observed six intensive lines of the molecules caused by rotational effects around of moments of inertia. As we see, there is a decrease of the value of frequencies of similar spectral lines. In a spectrum detrusion of frequencies depending on the sizes of crystallites is observed, the it is less particle size, the detrusion is more.

Intensity of lines of the molecules caused by rotational hunt effects around of an axis with the greatest moment of inertia also decreases with decrease of particle sizes. The same lines have also the greatest detrusion of frequencies. As we see, the modification of frequencies of lines even if it is a film and its size is observed varies in one direction. This film it is possible to consider as quasi a two-dimensional crystal. In a spectrum with decrease of width of a film appearance of additional lines of small intensity is observed. Intensity of these lines increases.

For an explanation of observable modifications of frequencies of lines calculations of spectrums of the lattice oscillations by a Dyne method [3] have been done. And calculations on transformation of parameters of a lattice at resizing crystallites. Minimization on energy was done for various layouts of molecules and their amount.

At matching the calculated spectrum with experimental it is discovered, that parameters of a lattice with decrease of the sizes of crystallites for para-dichlorbenzol are incremented. If to guess, that decrease of value of frequencies is linked only to decrease of the sizes of crystallites, how show calculations should be observed more significant decrease of frequencies for rotational oscillations linked with the least moment of inertia. The part of lines of small intensity can be caused by transmitting oscillations (these are lines in the field of 36 m⁻¹ and 70 m⁻¹) which intensity at decrease of width of a film is incremented. Appearance of additional lines can be caused by the several reasons that demands the further examination.

Thus, it is shown that at examination of films of organic crystals coming nearer to nanosized particle by a method of a Raman effect of light decrease of value of frequencies of the lattice oscillations is observed. As show calculations it is caused by magnification of parameters of a lattice of para-dichlorbenzol. As magnification of intensity of lines linked with transmitting oscillations is observed. The modification of physical properties because of resizing crystallites for the structures constructed of...
TABLE I: Modification of orientation oscillations frequencies with a modification of a film width.

| Film Width (µ cm⁻¹) | 22.5 | 43.5 | 45.5 | 49.5 | 91.0 | 100.0 |
|---------------------|------|------|------|------|------|-------|
| ~1µ               |      |      |      |      |      |       |
| ~5µ               | 25.8 | 45.5 | 47.5 | 53.5 | 92.0 | 100.5 |
| ~30µ              | 27.0 | 47.0 | 48.0 | 55.0 | 92.5 | 101.0 |

other organic molecules, probably, has other character.

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FIG. 1: A spectrum of the lattice oscillations of para-dichlorbenzol at resizing crystallites ~30µ, ~5µ and less 1µ.