MODELING OF OSCILLATORY STATES OF NANO-CRYSTALLINES WITH SUPERCOMPUTER MBC-1000

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A program complex for modeling of vibrations in crystallines of the given forms and sizes is designed. To resolve a vibrational problem a molecular approach is accepted. As a result we obtain a full harmonic vibrational spectrum of a crystalline. Only precision of model geometry and force constants as well as machine accuracy of computing procedures is limiting accuracy of spectral prediction. This enables to solve such lock-and-key problem for the mineralogy, as a role of surface and internal vibrations in the genesis of different polycrystalline forms of materials.

Program complex is intended for visual modeling of structure of elementary cell and real size crystalline on the personal computer. Hereinafter for crystallines with small cells calculations are led on PC as well, but for crystallines with complex elementary cells supercomputer MBC-1000 is used in the parallel calculations mode. Then crystalline vibrations are analyzed on PC in visual form.

We offer a necessary sequence of actions as well as corresponding algorithms for construction and processing of crystalline models.

For the true crystal cartesian coordinates of atoms and geometric parameters of elementary crystalline cell usually known from X-ray data. These coordinates are carried into special program Crystall.m, written in MatLab programming system. Chemical symbols of all atoms of cell as well as translation vectors are additional input data. Program translates each atom of entered elementary cell along the first translation vector. The program also traces overlappings of new atoms on of elementary cell frontier. Such atoms are rejected. We have got a pillar from two elementary cells. It is possible to repeat the process as many times as we need, assigning for a new model multiple size of translation vector. As a result we have got "1-D" crystalline chain. In this way it is possible to construct a spatial crystalline thread model. Such nano-threads are already obtained in the experiment, and their features are studied.

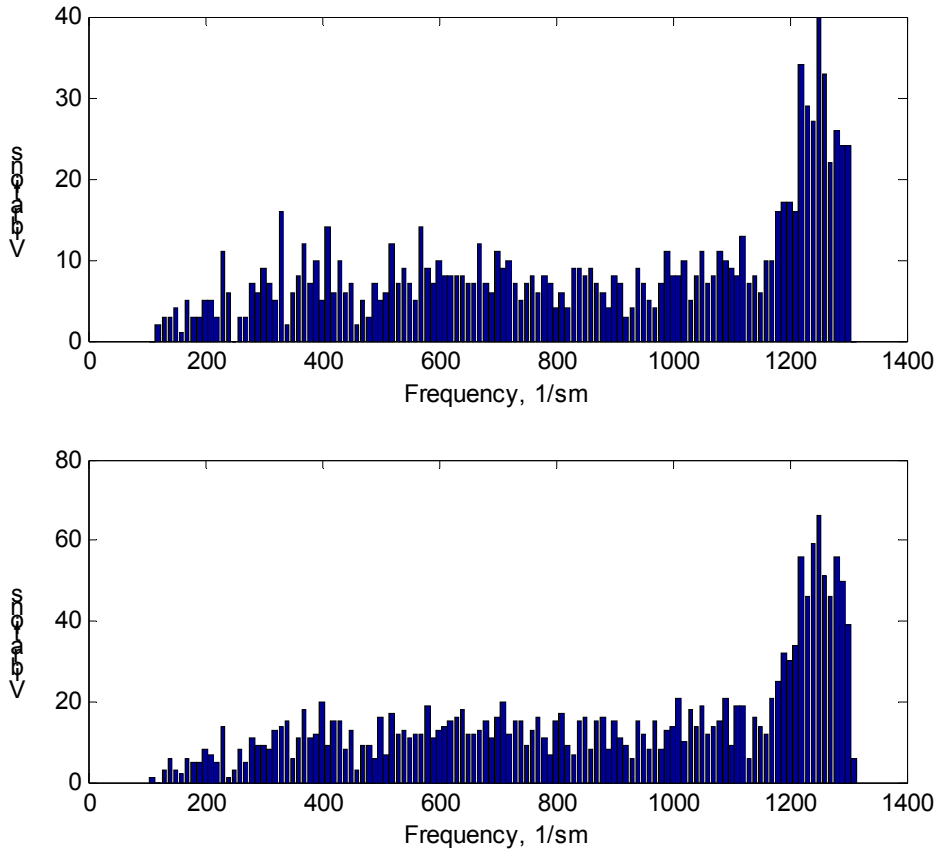
Hereinafter similar way "1-D " structure is translated in the second crystalline direction. Herewith we have got "2-D" model of superthin crystalline film. Such films present a grate interest for nanotechnique. Then a model of crystalline film is translated in the third direction. In total we have got crystalline model of any form and size. Unlike endless crystal models, such model has definitely denominated surfaces, to which it is possible to add films of other structure that it is required for modeling of surface reactions and phenomena of catalysis.

Having finished constructing a spatial crystalline structure, program analyses distances between atoms, finds minimum distances and for found thereby pares of atoms does necessary mark in a matrix of adjacency. This corresponds to possible chemical bonds in the crystal. On output a program creates a textual file. There are list of atoms and bonds in crystalline models in the file, then for each atom are written its cartesian coordinates and chemical symbol, then it is written matrix of adjacency by its upper triangle. This answers to the format of the files with the extension CT, in which contributes information on spatial structures of molecules known chemical modeling system ChemOffice. The researcher can use possibilities of ChemOffice to build necessary crystalline model, and export it in the external file in the given format. However, our program allows researcher sharply eliminate his labour, as far as it undertakes all operations on translations of elementary cell and on shaping a system of molecular bonds.

The special program using dependent coordinates forms vibrational Hamiltonian. Then it is automatically transforms it to the block form by means of transformations of symmetry. At resolving of eigenvalues and eigenvectors problem herewith appear zero own numbers. Their amount is an amount of linear dependencies between vibrational coordinates. We reject zero own numbers and corresponding eigenvectors. Dynamic part of the Hamiltonian is automatically formed by the program, which searches indicative force constant in molecular databases. This part of the Hamiltonian is transformed to new independent vibrational coordinates with aid of obtained system of eigenvalues and eigenvectors. Then we have got frequencies and forms of vibrational model by resolving of eigenvalues and eigenvectors problem for transformed force matrix. The forms of vibrations are described in the dependent vibrational coordinate system that vastly relieves an interpretation of

results. In the addition, forms of vibrations will be converted in cartesian shifts the atoms that allows to get visual animation of model vibrations.

As an example are brought results of the calculation of vibrations of diamond crystallines by the size of 4x3x3 and 4x4x4 elementary cells. On the picture histograms of frequencies in vibrational spectra of the crystallines are shown. Full spectrum of vibrational frequencies is depending on the size and form of diamond crystallines.



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