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COMPUTER MODELING OF DISSOCIATION PROCESS

Abstract. On the basis of the developed computer model this work studies the dynamics of molecular systems up to destruction (dissociation) by the example of triatomic molecules of nitrogen dioxide (NO_2).

Keywords: computer model, dissociation, Morse potential, chaotic vibrations.

Introduction

The possibilities of predictive modeling of material properties at the micro and nanoscale are closely related to the research of the dynamics of the molecular systems where the destruction is caused by the rupture of bonds between atoms of the substance. The dissociation of single molecules is an example of such destruction [1].

Statement of the problem

To develop the computer model of interatomic interaction at the level of molecular structure in the SimuLink environment based on molecular dynamics. On its basis study the specifics of the origin of chaotic vibrations and dissociation process. Get spectral characteristics of interatomic vibrations of separate phases of dissociation process by the example of nitrogen dioxide.

Main part

The modern conception of normal mode can actually explain many phenomena of molecular spectroscopy. However, it has a flaw in its basis, because of which you can not add the dissociation of chemical bonds at high excitation. Currently the adequate model that can describe the dissociation is Morse potential.

$$\Pi(r) = D\left[e^{-2\alpha(r-a)} - 2e^{-\alpha(r-a)}\right], \qquad (1)$$

The system of differential equations

$$\begin{cases} m_O \ddot{\underline{R}}_{O_1} = \underline{F}_{O_1N} + \underline{F}_{O_1O_2}, \\ m_N \ddot{\underline{R}}_N = \underline{F}_{NO_1} + \underline{F}_{NO_2}, \\ m_{O_2} \ddot{\underline{R}}_{O_2} = \underline{F}_{O_2N} + \underline{F}_{O_2O_1}. \end{cases} \qquad (2)$$

describes the dynamics of triatomic molecule NO_2. Under the conditions F_{ON1}, F_{NO1} , F_{ON2} , F_{NO2} , F_{O1O2} , F_{O2O1} – vectors of interaction force of atoms in a molecule. In particular

$$\underline{F}_{O_1N} = -\Pi'\left(R_{O_1N}\right)\underline{R}_{O_1N}/R_{O_1N}; \qquad \underline{R}_{O_1N} = \underline{R}_{O_1} - \underline{R}_N, \qquad R_{O_1N} = \left|\underline{R}_{O_1N}\right|, \qquad (3)$$

The model of triatomic molecule (2) was implemented in MatLab SimuLink. This has made it possible to obtain the results of calculations on a real time basis and currently, that is necessary to display model in Virtual Reality, for the purpose of obtaining three-dimensional images of the

dynamics of the molecule. Fig. 1 shows the first level of the constructed scheme.

The program has facilities of batch calculations of the dynamics of a model for different values of the initial energy. At the output it is possible to obtain the dynamics of vibration spectrum of each pair of atoms, dynamics of molecule's angles, dynamics of radius vectors of the atoms of the system.

As input parameters the program requires parameters of atoms (mass), their mutual arrangement, communication parameters (parameters of Morse potential) vectors of initial velocities of atoms and initial kinetic energy of the system as a whole. Such approach makes it possible to use the model for description of any triatomic molecules for which these parameters are known. The parameters that were used for NO_2 molecule are given in Table 1 [2].

Table 1 – parameters of model NO_2

Parameter	Hartree units
Mass of an atom of nitrogen	25529
Mass of an atom of oxygen	29176
Energy of a bond dissociation of N-O	0,179
Distance of a bond balance of N-O	2,249
Parameter α for a bond of N-O	1,122
Distance of a bond balance of O-O	4,138
Energy of a bond dissociation of O-O	0,0358
Parameter α for a bond of O-O	1,592

The scheme implements a system (2). The equations of a system are divided into blocks of the same type of forces, radius-vectors, equations. The system integrates over 100,000 cycles, at a pitch of 2.

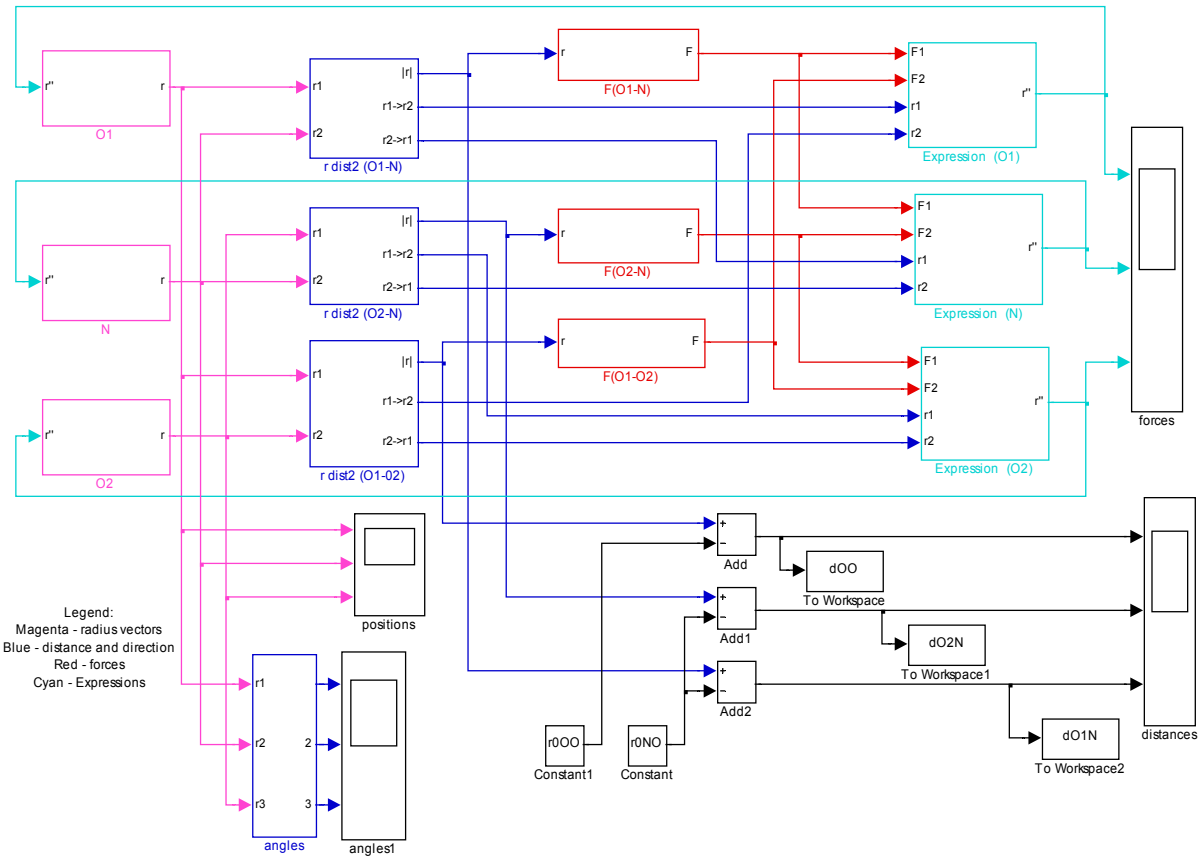

Figure 1 - The upper level of a model developed in SimuLink environment

It was obtained a system dynamics for NO_2 molecule for different values of the initial total energy of the molecule. Fig. 3 - 7 shows the vibrations and bond spectrum of O-O. The setting of kinetic energy is carried by the initial velocity of atoms:

$$V = \sqrt{\frac{2 \cdot Ek}{m}} \qquad (4)$$

Vector directions of velocity of atoms are calculated so that the sum of these vectors at the initial time becomes zero.

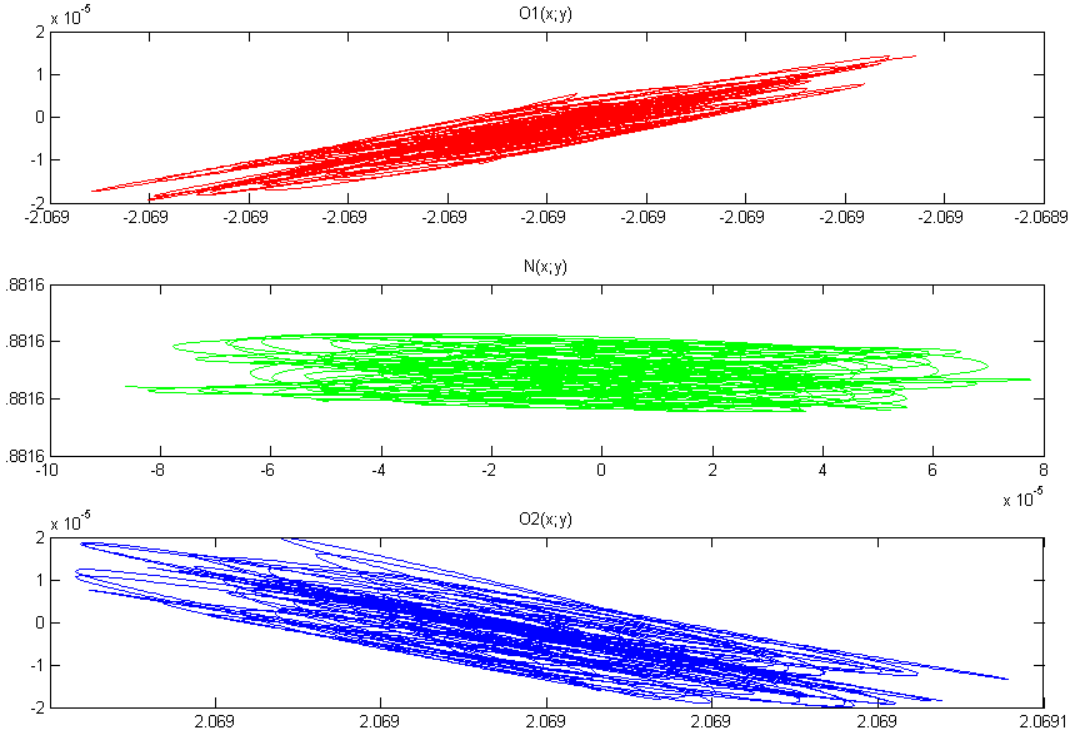

Figure 2 - Motion state of the atoms in the molecule NO_2 in 2D plane

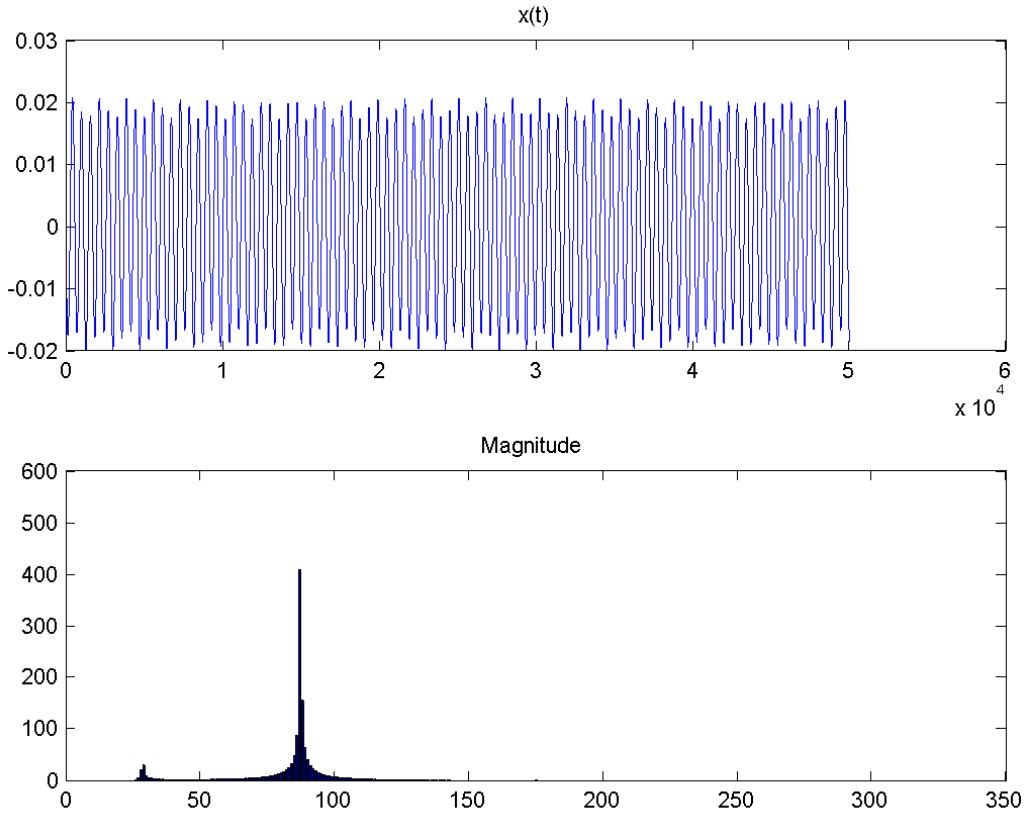

Figure 3 – Mode of vibrations O-O E_k=0,0001

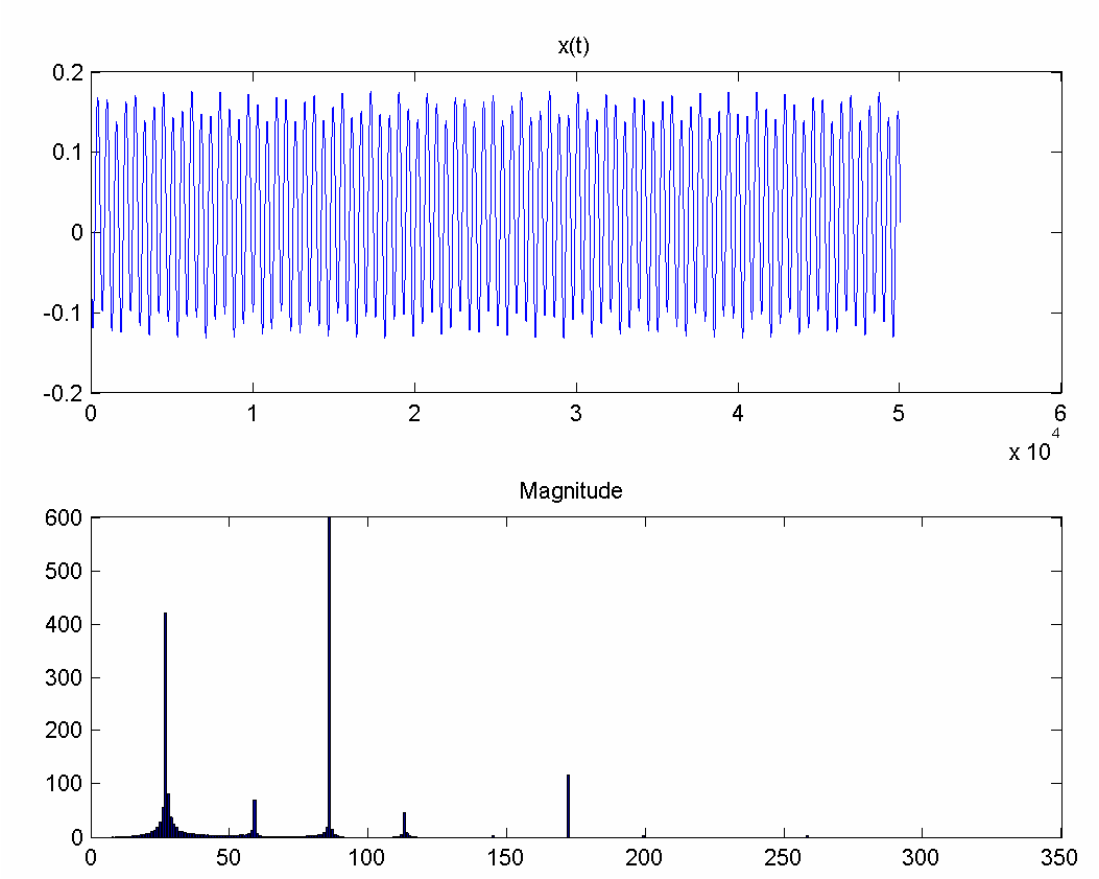

Figure 4 – Mode of vibrations O-O where E_k = 0,005

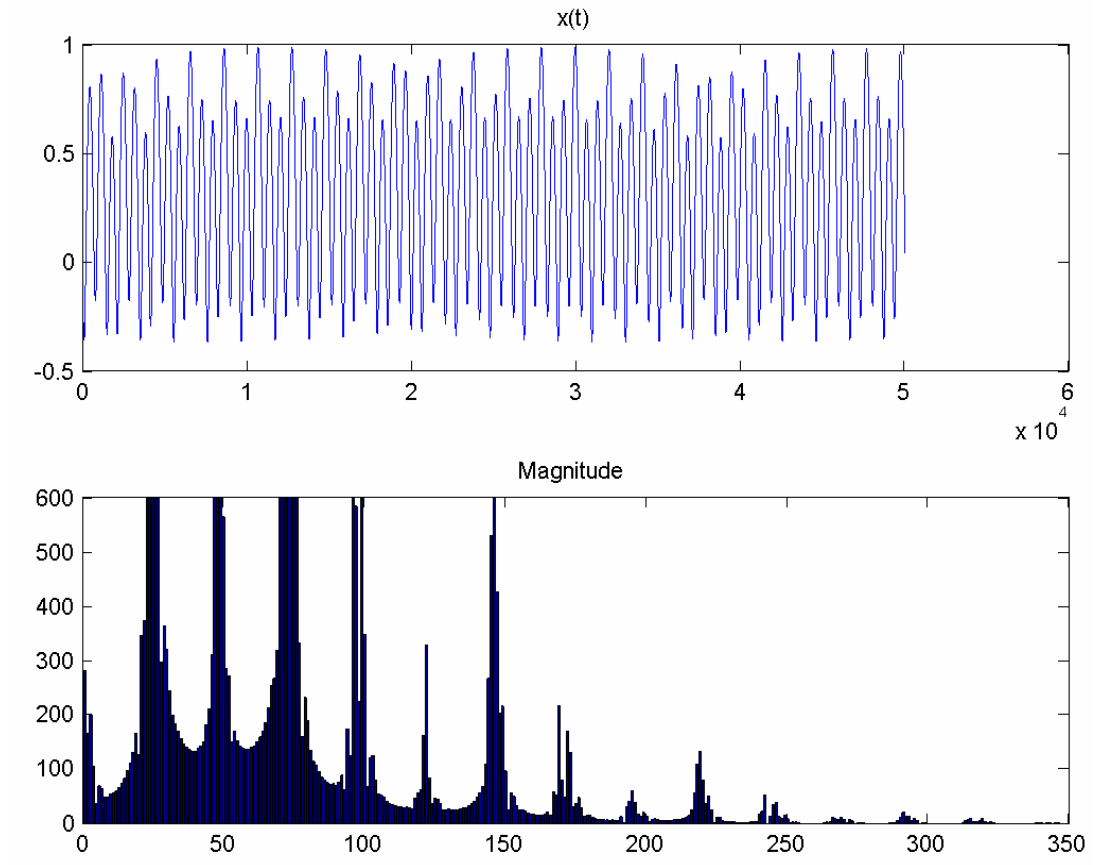

Figure 5 – Mode of vibrations O-O where E_k=0,06

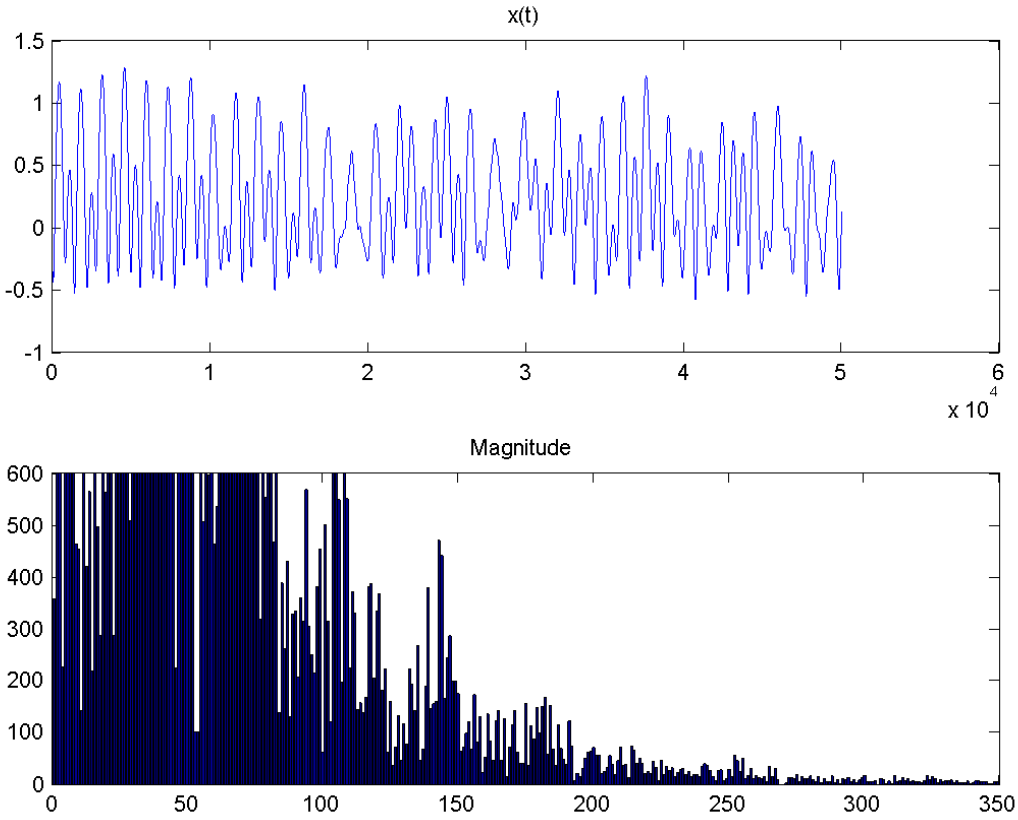

Figure 6 – Mode of vibrations O-O where Ek = 0,1

The dissociation energy in the case of NO_2 will be 3/2 of the energy of dissociation of the strongest bonds that is N-O. This is due to the fact that the total energy of the system is allocated to each atom of a system, and each bond is held only by two atoms. Figure 7 shows the mode of vibrations of bond O-O for the initial energy of the system close to the dissociation of the molecule.

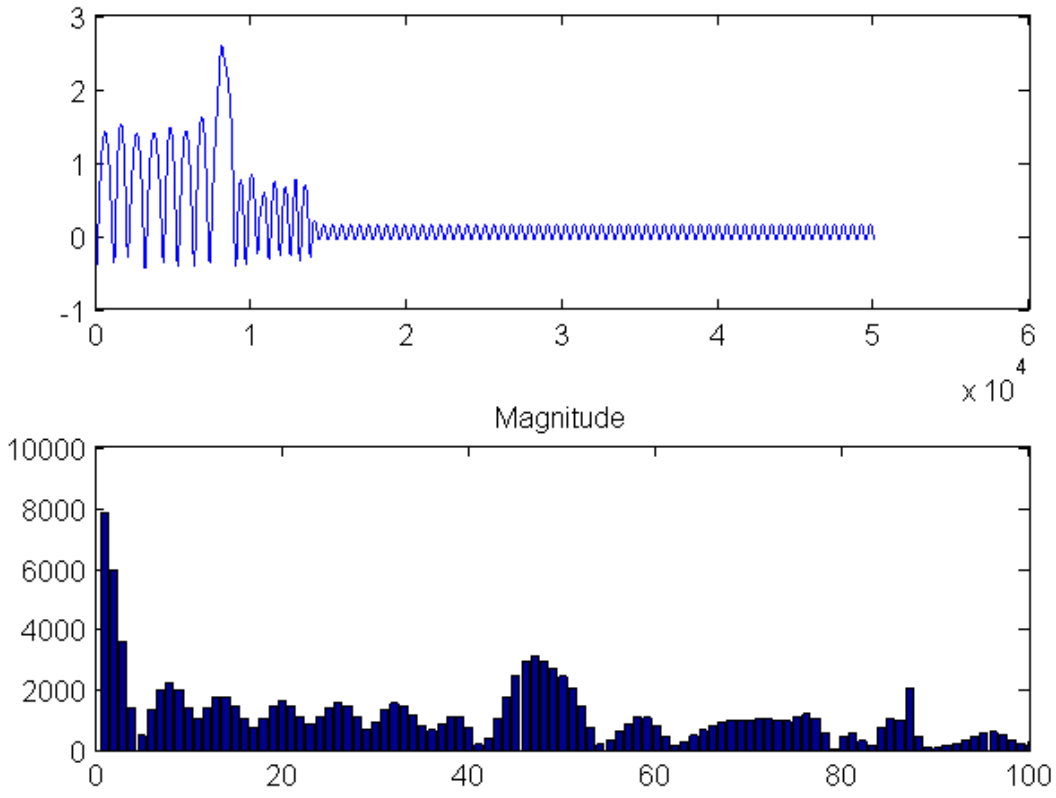

Figure 7 - Mode of vibrations O-O when E_k = 0,26

So there occurs a dissociation of both bonds that held the oxygen atom O_1. Complete dissociation has not occurred and it is shown in Fig. 7.

CONCLUSIONS

The computer model of interatomic interactions at the molecular structure and based on the molecular dynamics was developed in this work. This model allowed to undertake a study of the features of the origin of chaotic vibrations and dissociation process. By using the developed model there were defined the sequences of changes in the characteristics of dynamic model and changes of structure between atomic bonds, in case of the transition to chaotic vibrations. In general, the model can be used in a wide range of researches of interatomic interactions at the molecular structure bringing the obtained data to some extent the data obtained from physical experiments.

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