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IMAGING A NANOSTRUCTURE BY THE LYAPUNOV EXPONENT COMPUTATION

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Summary: A model of the AFM (atomic force microscope) with certain tip-nanostructure interaction, cantilever elasticity and damping of its oscillations is proposed. Stable and unstable motion of the AFM tip interacting with the graphene sheet is investigated by the Lyapunov exponent computation. In our approximation, a hundred Si atoms (top of the AFM tip) interact with C atoms of the nanostructure. This interaction is described by Lennard-Jones potential, and the distance between the top and the center of the cantilever mass is a constant. Complex influence of the initial tip-nanostructure distance and nanostructure size on stability has been examined. We discuss a possible new mode of the AFM operation based on the Lyapunov exponent computation. Maxima and minima of the Lyapunov exponent show where certain parts of the elementary cells are placed.

Keywords: AFM, nanostructure, Lyapunov exponent.

1. INTRODUCTION

Atomic force microscopy (AFM) serves as a tool for imaging surfaces with atomic resolution and surface atoms manipulation. AFM modes of operation are static (contact and non-contact) and dynamic (contact, non-contact and tapping). The mode is static if we measure deflection of the cantilever dragged across the sample surface. The mode is dynamic if we measure the cantilever amplitude, phase and frequency modified by tip-sample interaction. In contact mode, the surface atoms repulse the tip scanning the sample in close contact. In non-contact mode, the surface atoms attract the scanning tip 5-15 nm away. In tapping mode, or intermittent contact mode, the cantilever is driven to oscillate with the amplitude of 100-200 nm [1,2].

Nonlinear interaction between AFM tip and the sample that we investigate can lead to chaotic behavior [3-7]. We usually try to minimize instabilities in tip motion, but an AFM can be based on chaos, using local flow variation (LFV) method of time series analysis. LFV is a non-linear time series analysis method using phase space warping concept. Small changes of system parameters are related with feature vectors for chaotic and periodic motions. LFV characterizes changes of the probability distribution of trajectories in a subsystem phase space [8].

We propose here a model of AFM tip interacting with graphene and compute the Lyapunov exponent for different values of initial position and graphene size. The problem of stabilization and the possibility of a chaotic mode of operation will be considered.

2. THE MODEL

Motion of the AFM tip is influenced by interaction with graphene sheet, elastic force and damping. Graphene sheet containing $(2+2N)\cdot(4+4N)$ C atoms is placed in yz plane. The distance between the top of the AFM tip and the center of the cantilever mass is a constant. We solve the equation of the tip motion:

$$m\frac{d^2\vec{r}}{dt^2} = -\nabla U - \begin{bmatrix} \mu_x(x-\varepsilon x_0) \\ \mu_y(y-y_0) \\ \mu_z(z-z_0) \end{bmatrix} - \begin{bmatrix} \beta_x V_x \\ \beta_y V_y \\ \beta_z V_z \end{bmatrix} \quad (1)$$

Here m is mass of the cantilever containing $5\cdot10^{10}$ Si atoms (100 of them are interacting with the nanostructure), U is Lennard-Jones potential, describing interaction of Si and C atoms,

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$\mu_x = 4 \cdot 10^3$, $\mu_y = \mu_z = 2 \cdot 10^4$, $x_0 = x(0)$, $y_0 = y(0)$, $z_0 = z(0)$ (initial position of the top), $\varepsilon = 0.3$, $\beta_x = \beta_y = \beta_z = 0.1$ and V denotes velocity of the AFM tip. Units for time, distance, mass, force and spring constant are: $10^{-12}\,s$, nm, $10^{-27}\,kg$, $10^{-12}\,N$ and $10^{-3}\,N/m$. The top is above of its equilibrium position at $t = 0$ and elastic force moves the tip to the nanostructure.

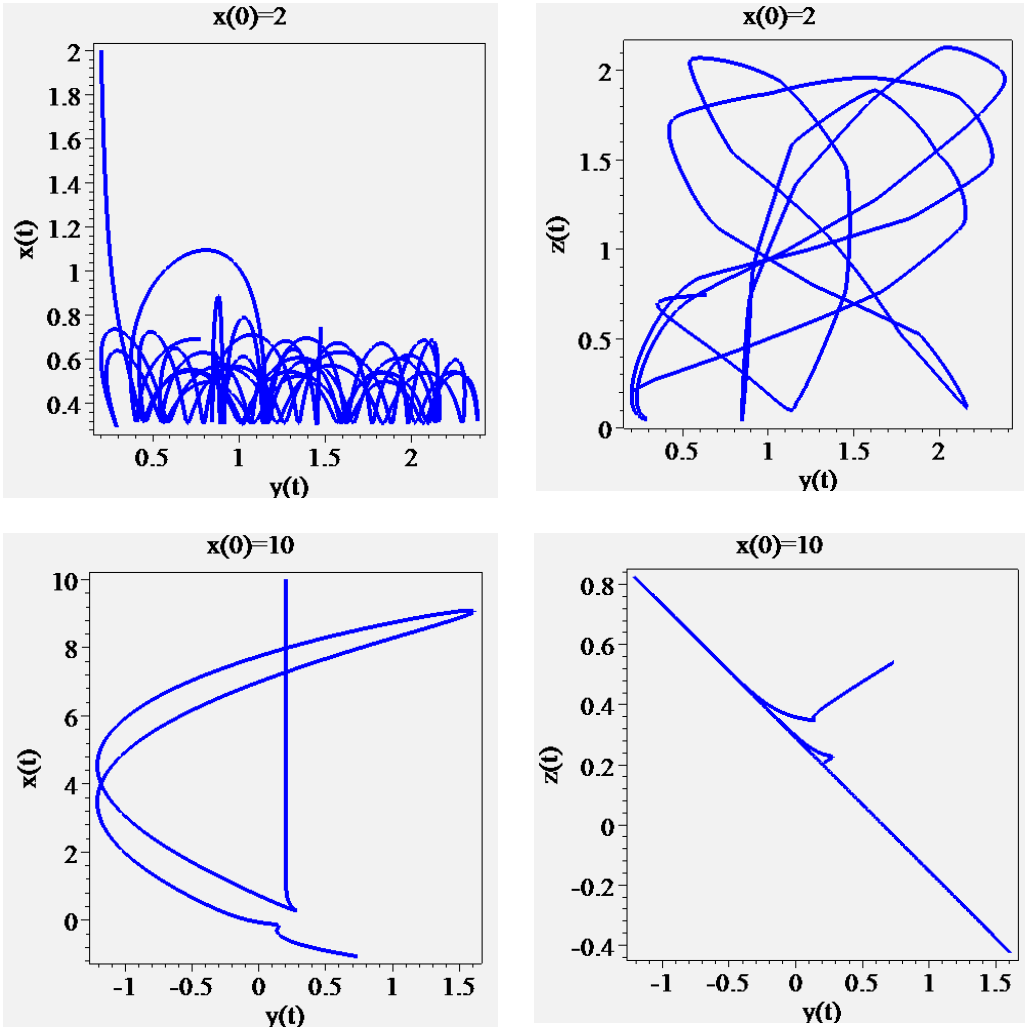

Figure 2.1. Motion of the tip is very complex if it is close to the nanostructure. Here $y(0) = z(0) = 0.2, N = 4$.

3. THE LYAPUNOV EXPONENT

In the analysis of some nonlinear systems with three or more dimensions strange things were observed with solutions or trajectories of the system whose initial or assumed solutions already exist, very little is different. What exactly was observed was that the difference in the two trajectories (solutions) grows exponentially with time, although the initial point of both two trajectories differ only negligibly. Growth rate differences determined the exponent L function which is known as the Lyapunov exponent. This phenomenon of rapid growth difference of two solutions to small changes in the initial point is called sensitivity to initial point. Specifically, a system is chaotic, if Lyapunov exponent is positive, i.e., greater than zero, and if the aperiodic behavior of the solution itself, otherwise the system is not chaotic. Sensitivity is necessary for the chaos, but not enough.

We consider time series $x(50j)$, where $j = 1,2,...,3000$, compute changes of $x(50j)$ ($j > 2800$) caused by small changes of $x(0)$, and find averaged Lyapunov exponent.

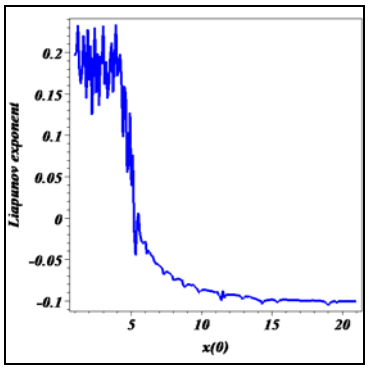

Figure 3.1. Dependence of the Lyapunov exponent on the initial tip-graphene distance with y(0)=1.4, z(0)=1.3 and N=3. The motion can be stabilized by increasing of the tip-nanostructure distance.

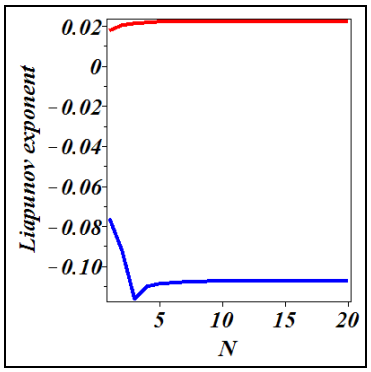

Figure 3.2. Dependence of the Lyapunov exponent on the nanostructure size with x(0)=21, y(0)=0.7, z(0)=0.6 (blue) and x(0)=18, y(0)=-0.1, z(0)=-0.1 (red).

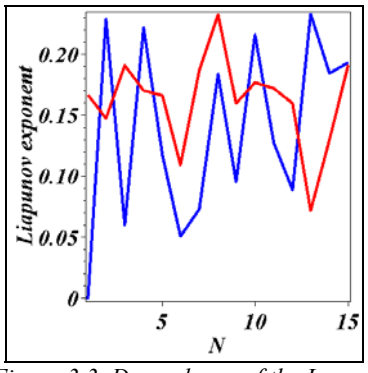

Figure 3.3. Dependence of the Lyapunov exponent on the nanostructure size with x(0)=4.2, y(0)=1.9, z(0)=-0.8 (blue) and x(0)=3.8, y(0)=1.5, z(0)=-0.4 (red).

4. IMAGING THE NANOSTRUCTURE

For certain values of $x(0)$, $z(0)$ and N we find values of the Lyapunov exponent in an interval of $y(0)$. Maxima and minima of the Lyapunov exponent show where certain parts of the elementary cells are placed. We find that AFM can be used in chaotic regime (positive Lyapunov exponent) as well as in regular regime (negative Lyapunov exponent).

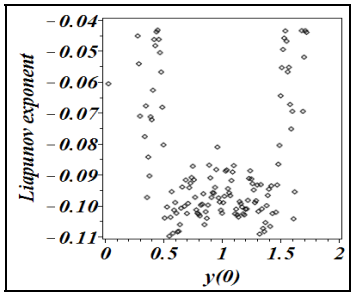

Figure 4.1. Lyapunov exponent with x(0)=18, z(0)=0.5 and N=2. The maximums at y(0) = 3a, 7a and 11a are showing positions of three hexagon centers (a=0.142 nm is the distance between neighbouring C atoms).

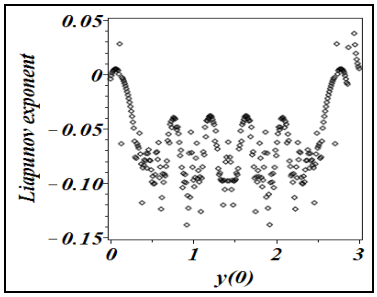

Figure 4.2. The Lyapunov exponent with x(0)=19, z(0)=0 and N=4. We can see two maximums on the edges and four maximums placed at y(0)= 6a, 9a, 12a, 15a.

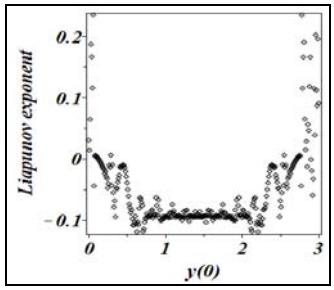

Figure 4.3. The Lyapunov exponent with x(0)=13, z(0)=1.136 and N=4. We can see two maximums on the edges and nine maximums showing central points between neighbouring C atoms.

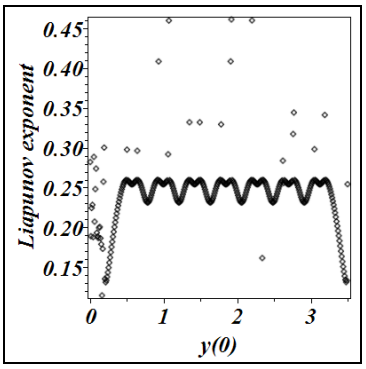

Figure 4.4. The Lyapunov exponent with x(0)=0.2, z(0)=3.3 and N=6. Maxima show positions of C atoms and minima show positions of hexagon centers. Considered oscillations are chaotic (Lyapunov exponent is positive).

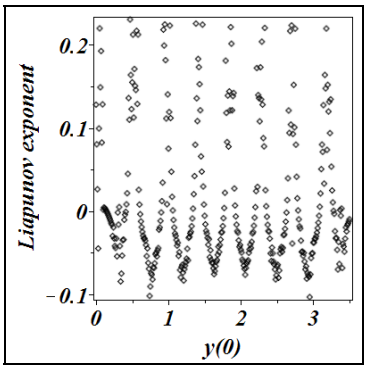

Figure 4.5. The Lyapunov exponent with x(0)=13.0, z(0)=3.3 and N=6.

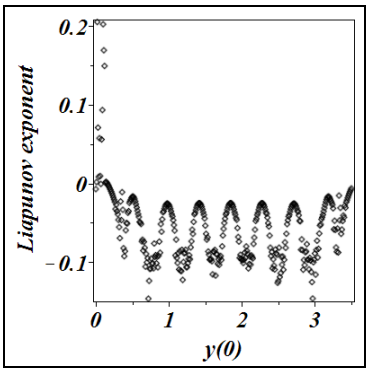

Figure 4.6. The Lyapunov exponent with x(0)=17.0, z(0)=3.3 and N=6

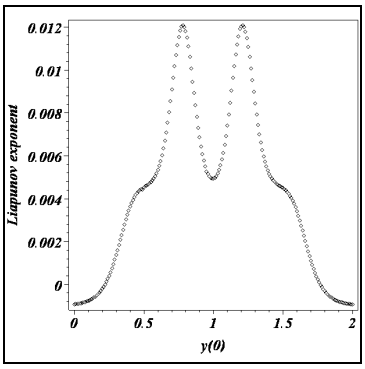

Figure 4.7. Here x(0)=30, z(0)=1.8, N=2.

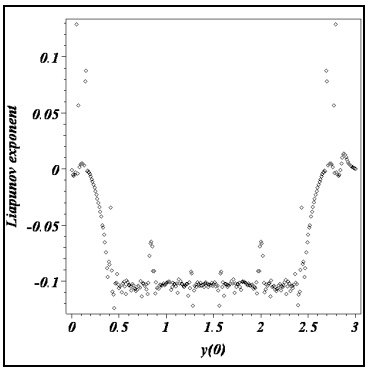

Figure 4.8. Here x(0)=30, z(0)=1.365, N=4.

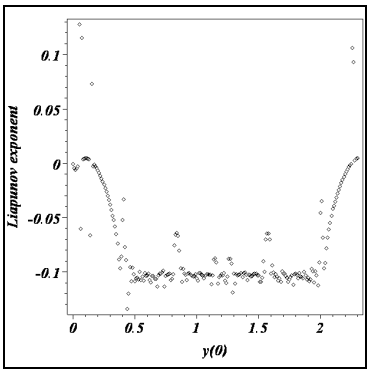

Figure 4.9. Here x(0)=30, z(0)=1.117, N=3.

5. CONCLUSION

Motion of the AFM tip is considered by computation, using a model where tip-nanostructure interaction, described by LJ potential, elastic force and damping are included. We find that the operation of AFM can be based on regular and chaotic oscillations of the tip and the Lyapunov exponent computation. Maxima and minima of the Lyapunov exponent show where certain parts of the investigated nanostructure elementary cells are placed. Stabilization is not necessary as in conventional approaches. Application of the proposed alternative AFM mode is very simple in comparison with LFV method presented earlier by Liu and Chelidze.

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ПРИКАЗИВАЊЕ НАНОСТРУКТУРЕ РАЧУНАЊЕМ ЉАПУНОВЉЕВОГ ЕКСПОНЕНТА

Сажетак: Предложен је модел АФМ-а (микроскоп атомских сила) са одређеним међудјеловањем шиљка и наноструктуре, одређеном еластичношћу носача и пригушењем његових осцилација. Истражено је стабилно и нестабилно кретање АФМ-овог шиљка који међудјелује са листом графена при чему се рачуна Љапуновљев експонент. У нашој апроксимацији, сто атома силицијума (врх АФМ-овог шиљка) међудјелује са угљениковим атомима наноструктуре. То међудјеловање је описано Ленард-Џонсовим потенцијалом а удаљеност врха од центра масе носача је константна. Размотрен је комплексан утицај почетне удаљености шиљка од наноструктуре и утицај величине наноструктуре на стабилност. Дискутирамо могућност новог начина функционисања АФМ-а који би био заснован на рачунању Љапуновљевог експонента. Максимуми и минимуми Љапуновљевог експонента показују гдје се налазе одређени дијелови елементарних ћелија.

Кључне ријечи: АФМ, наноструктура, Љапуновљев експонент.