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USING PERMUTATION ENTROPY FOR AFM DATA ANALYSIS

Dragana Malivuk[1], Saša Nježić[2], Sreten Lekić[1], Enes Škrgić, Zoran Rajilić[1,]*
[1] Banja Luka University, Faculty of Science, Mladena Stojanovića 2,
78000 Banja Luka, Republic of Srpska
[2] Banja Luka University, Faculty of Medicine, Save Mrkalja 14,
78000 Banja Luka, Republic of Srpska
[3] Gymnasium, 77220 Cazin, B&H

Abstract: We consider driven oscillations of the AFM cantilever in computational experiments. Complexity of motion is described by permutation entropy H(3), which we compute for data obtained during scanning. Our aim is to find the optimal values of the scanning velocity, initial position of the tip, and the driving force amplitude and frequency for imaging the nanostructure, in a specific dynamic mode of the AFM operation.
Keywords: AFM, permutation entropy, nanostructure.

1. INTRODUCTION

Permutation entropy is a complexity measure for time series [1]. This approach, based on comparison of neighboring values, can be used in the presence of observational and dynamical noise. The permutation entropy of order n is

$$H(n) = -\sum_{\pi} p(\pi)\log p(\pi) \qquad (1)$$

where $p(\pi)$ is relative frequency of permutation π. The logarithm base is 2. If $n = 2$, there are two permutation types: $x_t < x_{t+1}$ and $x_t > x_{t+1}$. If $n = 3$, there are six permutation types: $x_t < x_{t+1} < x_{t+2}$, $x_{t+1} < x_t < x_{t+2}$, $x_{t+2} < x_t < x_{t+1}$,

Here we compute $H(3)$ for the data obtained in computational experiments with AFM, a tool for imaging surfaces with atomic resolution [2]. AFM modes of operation are static (contact and non-contact) and dynamic (contact, non-contact and tapping).

Different AFM modes (phase shift imaging, atomic force acoustic microscopy, force spectroscopy) are applicable to mapping the distribution pattern of low-molecular-weight biomimetic groups on polymer biomaterial surfaces [3]. Amplitude modulation AFM in air has application to high-resolution imaging of macromolecular complexes [4]. High-speed mapping of the elastic properties of various structures in air is performed using high bandwidth interdigitated AFM probes [5].

In a specific dynamic mode of the AFM operation, that we consider here, the cantilever performs driven oscillations. The optimal values of the scanning velocity, initial position of the tip interacting with a nanostructure, and the driving force amplitude and frequency will be determined.

2. THE MODEL

We solve the equation of the AFM tip motion:

$$m\frac{d^2\vec{r}}{dt^2} = -\nabla U - \begin{bmatrix} \mu_x(x-x_0) - A\cos\omega t \\ \mu_y(y-y_0-V_{scan}t) \\ \mu_z(z-z_0) \end{bmatrix} - \beta\vec{V} \qquad (2)$$

where $m = 2.324\cdot 10^{-15}kg$ is mass of the cantilever, $\vec{r}$ shows the position of the top, U is Lennard-Jones potential, $\mu_x = 4\frac{N}{m}$, $\mu_y = \mu_z = 20\frac{N}{m}$, (x_0, y_o, z_0) is initial position of the top, V_{scan} is scanning velocity, A is amplitude of the driving force, ω is frequency of the driving force, $\beta = 10^{-16}\frac{Ns}{m}$, and $\vec{V}$ is velocity of the AFM tip. The Lennard-Jones potential describes interaction of the tip with a few atoms placed on y axes, in their equilibrium positions. Scanning velocity has y direction.

We compute permutation entropy $H(3)$ of time series $x(t+nh)$, where $h = 10ps$ and $n = -249, -248, \ldots, 250$. Certain value of permuta-

* Corresponding author: ZoranRajilic@netscape.net

tion entropy is assigned to a very small part of the observed structure. Corresponding displacement of the AFM tip, in y direction, is $\Delta y = 500hV_{scan} \approx 0.01nm$.

3. RESULTS

For appropriate values of the initial tip-structure distance $x(0)$, scanning velocity V_{scan} (in y direction), amplitude of driving force A and frequency of driving force ω, the permutation entropy picks are at the atom places.

First we investigate complexity of the AFM tip motion when it interacts with four atoms placed on y axes at 0, 0.15, 0.3 and 0.45, for different values of the initial tip-structure distance (fig. 1). Next we find out the optimal scanning velocity of the tip interacting with atoms at 0, 0.15, 0.35 and 0.5 (fig. 2). Then we consider different values of A and ω (fig. 3, fig. 4). Permutation entropy can be changed significantly at small changes of the frequency ω.

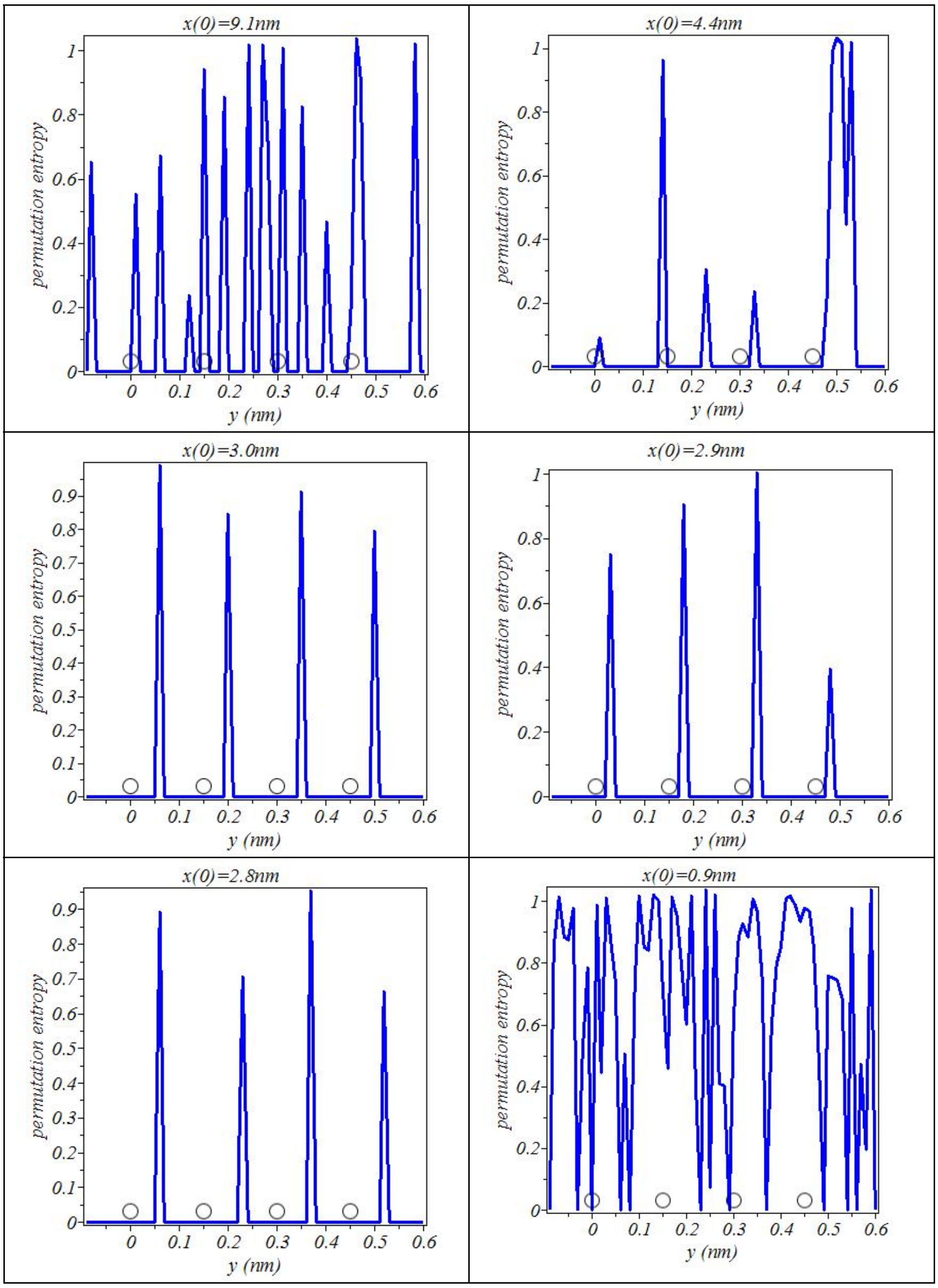

Figure 1. For $y(0) = -0.1nm$, $z(0) = 0$, $V_{scan} = 2mm/s$, $A = 9pN$ and $\omega = 3THz$, the optimal value of $x(0)$ is $2.9nm$. Circles denote the places of atoms

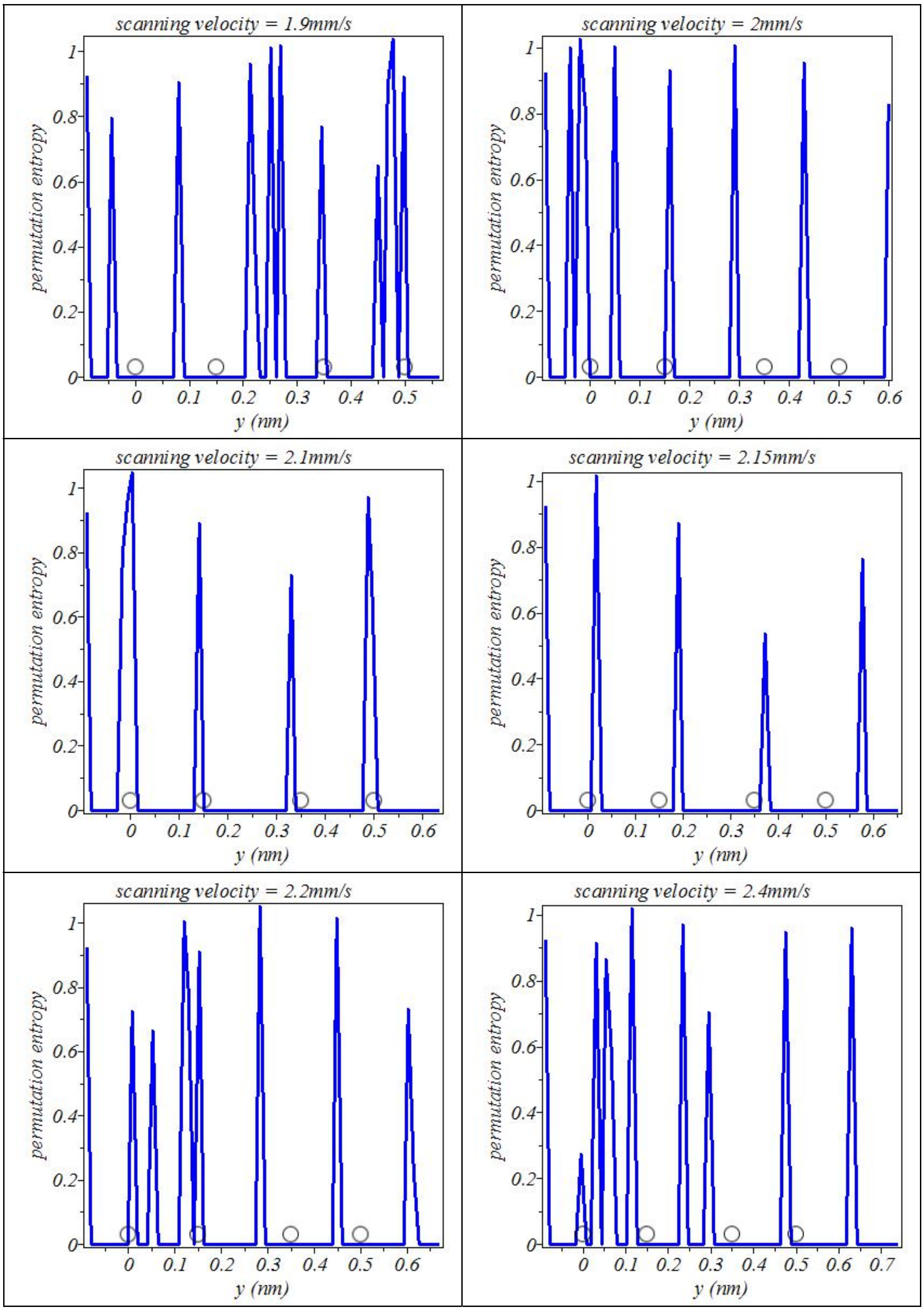

Figure 2. For $x(0) = 41nm$, $y(0) = -0.1nm$, $z(0) = -0.02nm$, $A = 55pN$ *and* $\omega = 3.1THz$, *the optimal value of* V_{scan} *is* $2.1mm/s$

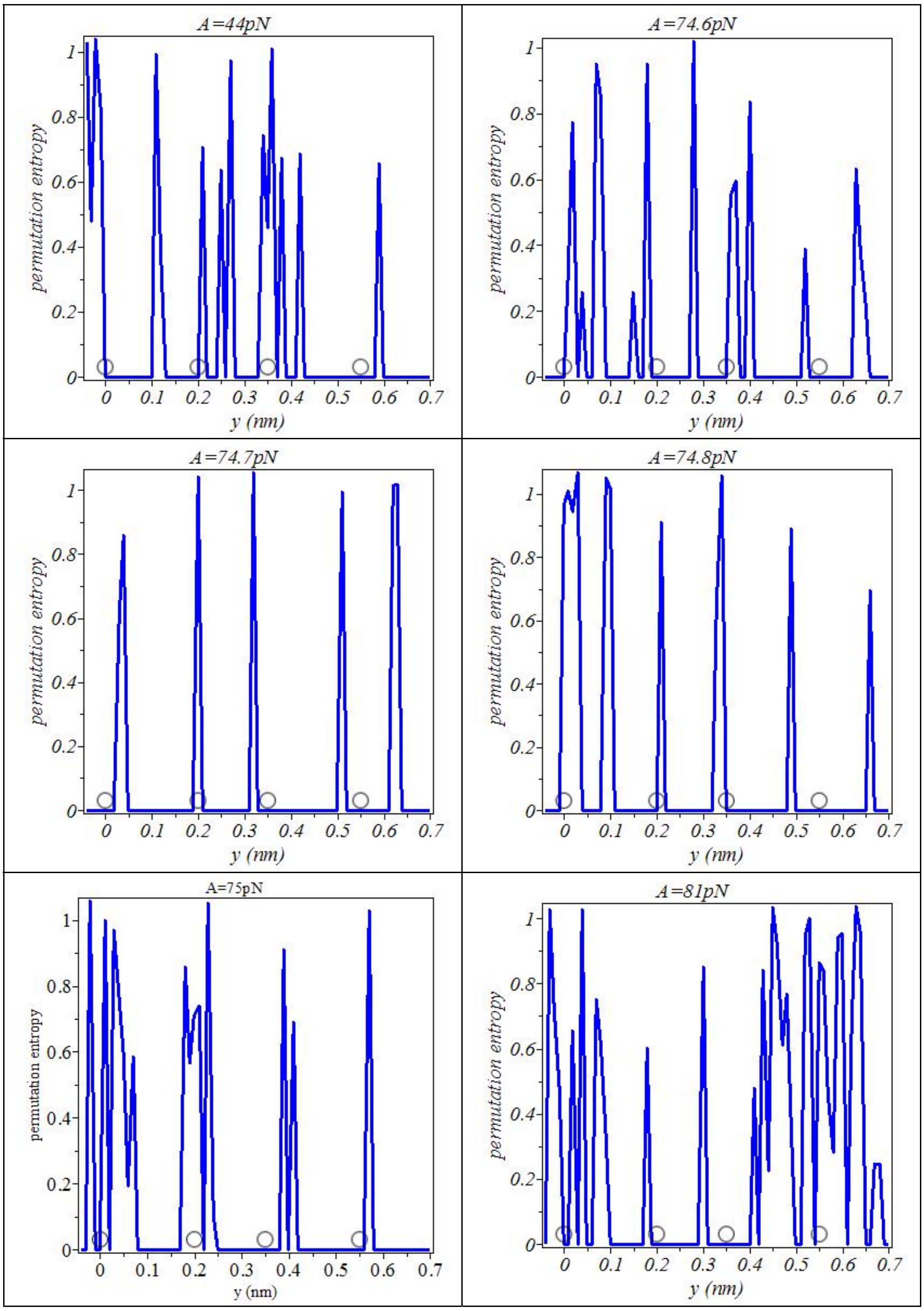

Figure 3. For $x(0) = 3.4nm$ *,* $y(0) = -0.05nm$ *,* $z(0) = 0$ *,* $V_{scan} = 2mm/s$ *and* $\omega = 3THz$ *, the optimal value of* A *is* $74.7\,pN$

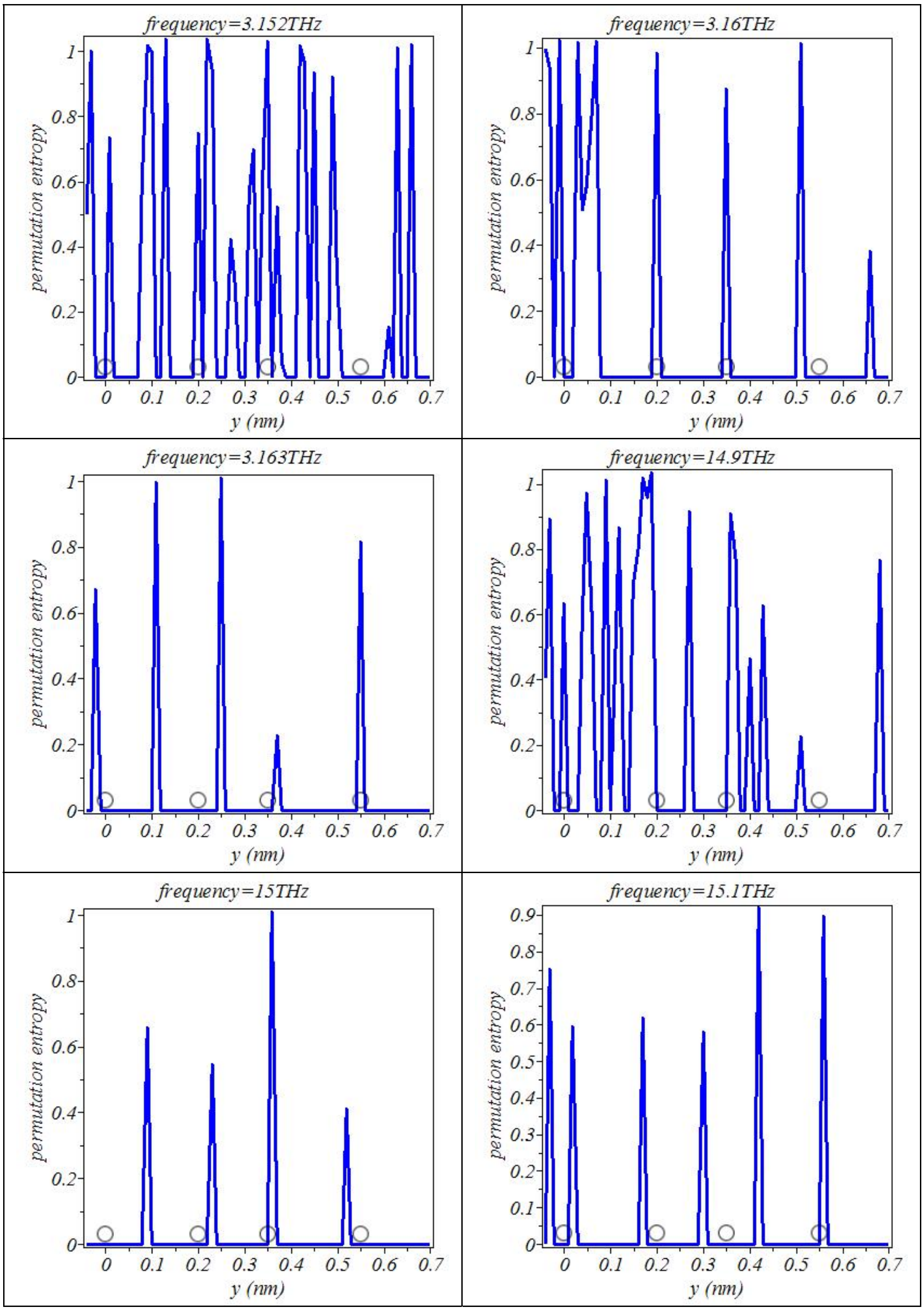

Figure 4. If $x(0) = 3.2nm$, $y(0) = -0.05nm$, $z(0) = 0$, $V_{scan} = 2mm/s$ *and* $A = 11pN$, *it is very difficult to find out an appropriate value of frequency* ω. *If* $\omega = 15THz$, *three picks are approximately at the atom places*

4. CONCLUSION

Driven oscillations of AFM cantilever are considered in computational experiments. For appropriate values of the initial tip-structure distance, scanning velocity, amplitude of the driving force and frequency of the driving force, imaging of a nanostructure using permutation entropy is possible.

5. REFERENCES

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КОРИШЋЕЊЕ ПЕРМУТАЦИОНЕ ЕНТРОПИЈЕ ПРИ АНАЛИЗИ ПОДАТАКА ДОБИЈЕНИХ ПОМОЋУ АФМ-а

Сажетак: У рачунарским експериментима посматрамо принудне осцилације носача шиљка АФМ-а (atomic force microscope). Комплексност кретања описана је пермутационом ентропијом H(3), коју рачунамо за податке прикупљене при скенирању. Циљ је пронаћи оптималне вриједности брзине скенирања, почетног положаја шиљка као и амплитуде и фреквенције принудне силе за приказивање наноструктуре, у једном специфичном динамичком моду рада АФМ-а.

Кључне ријечи: АФМ, пермутациона ентропија, наноструктура.