Nanoscale physics

Numerical Modeling the Rayleigh Instability of Ultrathin Metal Nanorods

V.N. Gorshkov, **D.V. Savchenko**

National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Prospect Peremohy, 37, Kyiv-03056, Ukraine.
E-mail: vn.gorshkov@gmail.com

The fragmentation of nanowires at temperatures lower than the melting point was investigated in detail in a number of experimental works [1,2]. The fragmentation mechanism is similar to Rayleigh instability [1] that spontaneously develops in liquid jets under the action of surface tension forces. In nanowires, this effect can be realized by the surface diffusion of atoms. The determination of the statistical characteristics of such a fragmentation process is an important task for the practical applications of the instability considered since a reliable control over this instability process can provide an effective, powerful, and economical technique for patterning self-assembled nanosphere chains on a relatively large scale by using Au nanowires as a starting point [1]. In our work, we present the investigation of the dynamics of nanorods based on the statistical mesoscopic model on the assumption that all the atoms (internal and surface ones) are located at the sites of FCC lattice, which is typical for many metals. We have determined the features of the fragmentation process under different temperature conditions and its mechanisms, related to nanorods limitations. In addition we have explained the series of experimental results, obtained in previous works. The work is supported by Ministry of Education and Science of Ukraine (Project F2904).

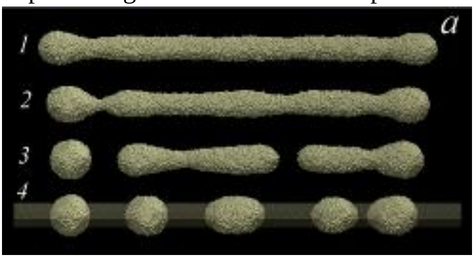

Fig. 1. *The shape dynamics of limited nanoroad in time (4 - the initial shape is shown by faded color).*

1. *Karim S., Toimil-Molares M. E., Balogh A.G., Ensinger M., Cornelius T. W., Khan E. U., Neumann R.*. Morphological evolution of Au nanowires controlled by Rayleigh instability // Nanotechnology.-2006.-**17.**-P. 5954-5959.
2. *Takahata R., Yamazoe S., Warakulwit C., Limtrakul J., Tsukuda T.* Rayleigh Instability and Surfactant-Mediated Stabilization of Ultrathin Gold Nanorods // J. Phys. Chem. C.-2016.-**120.**-P. 17006-17010.