「様式３」

Project No.：2077

Formation of a quasiperiodic relief on vicinal surfaces

［１］Organization
Project Leader：
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Olga Lisina, Ph.D. (V. N. Karazin Kharkiv National University, Ukraine)

［２］Research Progress

The aim of the project was to study the processes leading to the formation of a quasiperiodic relief on the vicinal surface of the crystal during layered growth from the vapor. The structure and behavior of nonlinear density waves of elementary steps on thermodynamically stable vicinal surfaces have been described, in the case when dissipative effects prevail over dispersion ones. The periodicity is a key requirement for creation of low-dimensional structures (quantum wells, quantum wires, quantum dots, etc.) used in optoelectronic and microelectronic devices.

The project participants actively collaborated with each other by providing the information through electronic media and face-to-face when the Ukrainian partners *O. Kulyk* and *O. Podshyvalova* visited RIE, Hamamatsu in January 2020 (research visits in the frame of the 2019 Cooperative Research at Research Center of Biomedical Engineering). They reported the obtained results, exchanged the data and ideas on join research in frames of the collaborative project, and discussed the issues of further cooperation between the partner institutions.

Apart from achieving the research results, described in the next section, the project participants were involved in the holding of the international scientific forums in Ukraine to discuss the research work concerning the project topics and general cooperation issues.

Dr. O. Kulyk presented the project-related results at The Int. Scientific and Technical Conf. "Physical and Technical Problems of Energy and Their Solutions 2019" (Kharkiv, Ukraine, 19 Jun. 2019) [1,2], The 18th Int. Conf. on Global Research and Education in Engineering for Sustainable Future, Inter-Academia 2019, (Budapest, Hungary 4-7 Sep. 2019) [3] and submitted the abstract with the key research findings to the Book of Abstracts of The Annual Meeting of 2019 Cooperative Research on Biomedical Engineering (Yokohama, Japan, 13 Mar. 2020) [6].

Totally, 6 publications (2 articles and 4 abstracts) have been published during the project implementation [1-6].

［３］Results

（３－１）Research results

The averaging method on large intervals of spatial coordinate change, which nevertheless remained infinitely small, was used to derive the Korteweg-de Vries-Burgers (KdV-B) equation for an one-dimensional (1D) step model on a vicinal surface of a crystal [4]. The microscopic approach is based on solving the Burton, Cabrera and Frank equations for the one-dimensional motion of a diffusion-coupled system of elementary steps. The qualitative picture of the phenomena depends on the competition of nonlinear processes with dissipative and dispersion effects determined by higher derivatives in the KdV-B equation. In the case when dissipative effects prevail over dispersion effects, the KdV-B equation transforms into the well-known Burgers equation. Such transformation is possible due to the smallness of the characteristic parameter, which is proportional to the ratio of the perturbation wavelength to the dimensionless density (i.e. the concentration of steps in the initial state of the vicinal surface).

1. Using computer modeling, the numerical solution of the one-dimensional non-stationary Burgers equation with periodic initial conditions was obtained [6]. The equation solving was performed with a meshless scheme using the method of partial solutions and radial basis functions. The time discretization of the one-dimensional Burgers differential equation was carried out by the generalized trapezoidal method. The inverse multiquadric function was used as radial functions. The solution of the one-dimensional non-stationary Burgers equation is visualized as a three-dimensional surface plot (Fig. 1). Qualitative analysis of the solution in the form of three-dimensional plots for individual time intervals indicates that over time there is an increase in the slope of the wave profile, which describes the dimensionless density of steps. In relation to the normalized profile of the vicinal surface for the 1D-step model, this means a redistribution of the concentration of steps.

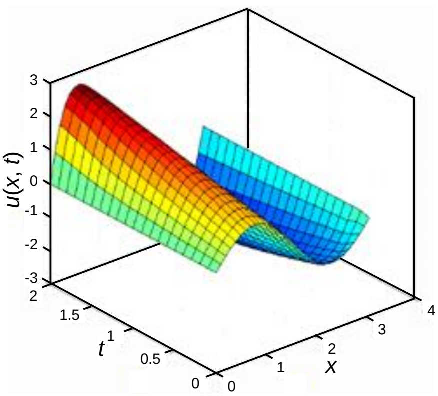

Fig. 1. A numerical solution of the Burgers equation with periodic initial conditions: *u*(*x*, *t*) is the velocity of the wave profile, *x* and *t* are the coordinate and time, respectively.

2. For quantitative analysis and interpretation of the experimental data, the analytical solution of the one-dimensional non-stationary Burgers equation with periodic initial conditions was obtained for the first time:

$$u(t,x) = 2\mu\lambda_n \frac{\sin(\lambda_n x) C_R e^{\mu\lambda_n^2 t}}{\left(\cos(\lambda_n x) + C_R e^{\mu\lambda_n^2 t}\right)^2 + \left(\sin(\lambda_n x)\right)^2}, \quad (1)$$

where $\lambda_n = 2\pi n, n = 1, 2, 3...$ are integers.

Solution (1) for $n = 1$ is visualized as a three-dimensional surface plot (Fig. 2). The feature of the obtained solution is the possibility to predict the discontinuity of the step concentration, which corresponds to the process of shock kinematic wave formation on an initially atomically smooth vicinal surface. In the case $n \geq 2$, at some stage of the process, one can observe a set of alternating shock waves similar to $n = 1$, which determines a quasiperiodic macrostep surface topography.

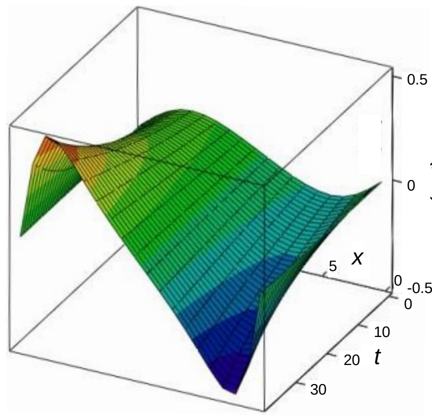

Fig. 2. An analytical solution of the Burgers equation with periodic initial conditions, which demonstrates the tendency of the wave profile to a sawtooth shape.

3. The described surface topography was found on the vicinal NaCl surface (near (100)) for step bunches with orientations [10] and [01] during growth from the vapor phase (Fig. 3).

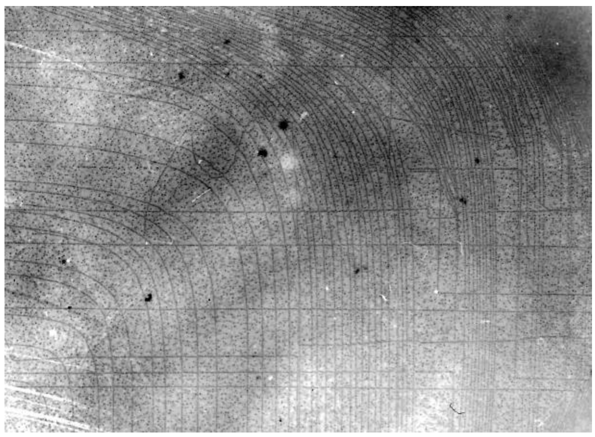

Fig. 3. TEM image of the vicinal growth surface near (100) NaCl formed during the pore motion in the temperature gradient.

The area shown in Fig. 3 is a part of the growth surface of a pore that was moving in the crystal due to the temperature gradient [4]. The supersaturation that occurs inside the pore near the growth surface as well as the characteristic parameters of the surface morphology indicate that the observed kinematic waves should be described exactly by the Burgers equation (not by KdV-B). Unfortunately, the used technique of electron microscopic vacuum decoration does not allow us to specify the distribution of elementary steps within the observed macrosteps. However, it makes possible to determine the number of elementary steps involved in the formation of step-bunch structures, which we call macrosteps. Such determination of the number of elementary steps is possible because elementary steps with a direction of the <11> type practically do not form step-bunch structures. Apparently, this morphological difference is due to the fact that the kinetic coefficients of the elementary steps of the direction <11> are much more than ones of the <10> steps.

4. To describe the experimental results with our analytical solution of the one-dimensional non-stationary Burgers equation with periodic initial conditions, we carried out the following:

- digitized the selected surface area for 75 elementary steps in the [10] and [11] directions;
- reproduced the topography of the investigated surface area;
- basing on the obtained data and known values of the length of adatoms diffusion path [4], the dependences of the step concentration on the longitudinal coordinate in the [10] direction were constructed (markers in Figs. 4 and 5).

It was shown that waves with small amplitudes (1 and 2 on the left side in Fig. 4) and waves with large amplitudes (step-bunch structures of different heights 3-5 on the right side in Fig. 4) move towards each other.

5. The experimental dependences of the concentration of steps on their coordinate were approximated by theoretical curves based on solution (1) (solid lines in Fig. 5) using the software Origin Pro and Matlab. Adequate agreement between the theoretical calculations and experiment allowed us to determine the values of the characteristic parameters of the observed shock waves.

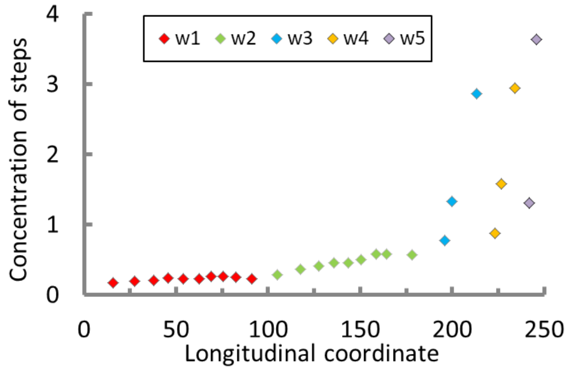

Fig. 4. Dependence of the step concentration on the longitudinal coordinate in the direction [10] (the concentration of steps for waves 2-5 was determined by averaging over several adjacent terraces; for convenient approximation of the results, the same direction of the waves was chosen).

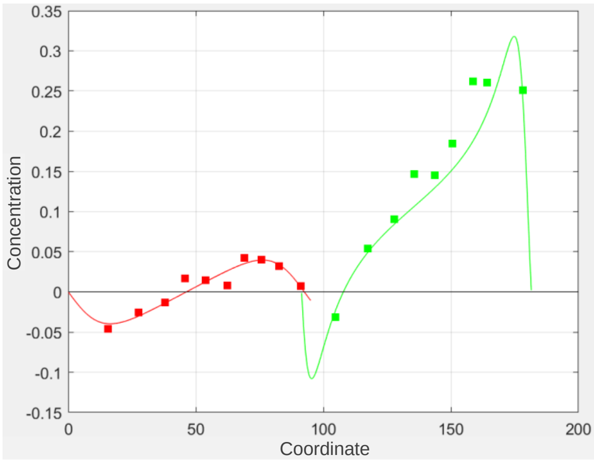

Fig. 5. Structure of the shock waves (1 and 2) shown in Fig. 3: marks indicate the values of monatomic steps concentration; solid curves demonstrate the result of the computations based on equation (1).

(3 – 2) Ripple effects and further developments

The obtained research results and calculated data on the characteristic parameters of the considered shock waves open up the possibility of an analytical solution of the problem on the formation of a quasi-periodic relief on thermodynamically stable vicinal surfaces under nonequilibrium conditions. In particular, it becomes possible to describe the kinetic regularities of the formation of the quasiperiodic surface profile shown in Fig. 6. As known, periodicity is the main requirement for obtaining low-dimensional structures.

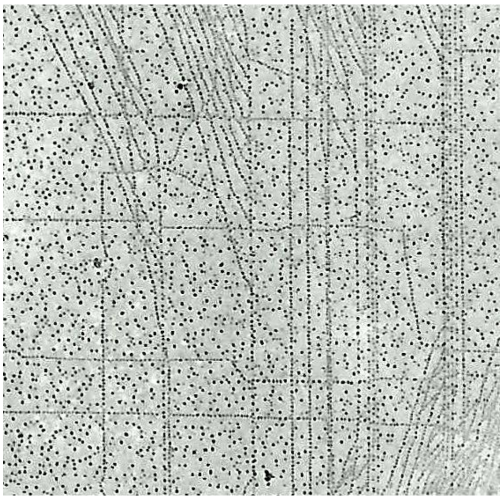

Fig. 6. TEM image of a quasiperiodic relief formed on the pore growth surface near (100) NaCl (macrosteps are represented by elementary step bunches; broken and rectilinear steps intersecting the step bunches are slip bands that appeared when the crystal was split and the pores were opened in vacuum before the procedure of decorating with gold particles).

［4］Achievements (List of Publications)

(1) O.P. Kulyk, V.I. Tkachenko, O.Yu. Lisina, V.O. Mikhnych, V.A. Gnatyuk, T. Aoki, Nonlinear effects of diffusion interaction of steps on thermodynamically stable vicinal surfaces, *Physical and Technical Problems of Energy and Their Solutions 2019, Proceedings of the International Scientific and Technical Conference*, P. 13, 2019 (Kharkiv, Ukraine, 19 June 2019). (*Plenary report*)

(2) V.M. Kolodyazhny, O.P. Kulyk, O.Yu. Lisina, Approximate solution of the non-stationary Burgers-Korteweg de Vries' problem based on the use of a generalized Taylor series, *Physical and Technical Problems of Energy and Their Solutions 2019, Proceedings of the International Scientific and Technical Conference,* P. 48, 2019 (Kharkiv, Ukraine, 19 June 2019). (*Plenary report*)

(3) O.P. Kulyk, L.A. Bulavin, S.F. Skoromnaya, V.I. Tkachenko, Model of induced motion of inclusions in the field of forces of an inhomogeneously stressed crystal, *The 18th International Conference on Global Research and Education in Engineering for Sustainable Future, Inter-Academia 2019, Program and Book of Abstracts*, P. 9-10, 2019. (4-7 September 2019, Budapest and Balatonfüred, Hungary).

(4) O.P. Kulyk, V.I. Tkachenko, O.V. Podshyvalova, V.A. Gnatyuk, T. Aoki, Nonlinear interaction of macrosteps on vicinal surfaces at crystal growth from vapour, *Journal of Crystal Growth*, Vol. 530, P. 125296-1-7, Jan. 2020. *DOI: 10.1016/j.jcrysgro.2019.125296*

(5) O.P. Kulyk, L.A. Bulavin, S.F. Skoromnaya, V.I. Tkachenko, Model of induced motion of inclusions in the field of forces of an inhomogeneously stressed crystal, *in: A.R. Varkonyi-Koczy (ed.) Engineering for Sustainable Future. Inter-Academia 2019. Lecture Notes in Networks and Systems (LNNS)*, Vol. 101, P. 326-3397, 2020, Cham: Springer. *DOI: 10.1007/978-3-030-36841-8_32*

(6) O. Kulyk, I. Hariachevska, O. Lisina, V. Tkachenko, O. Andrieieva, O. Podshyvalova, V. Gnatyuk, T. Aoki, Formation of a quasiperiodic relief on vicinal surfaces, *The Annual Meeting of 2019 Cooperative Research on Biomedical Engineering, Book of Abstracts*, Abstract No 1-11, 2019, (13 March 2020, Tokyo, Japan), *in press.*

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Travelling Report (Mention each travel by CRP budget.)

Name : Oleksandr Kulyk

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Period of time : 04 January – 20 January 2020

Destination : Research Institute of Electronics, Shizuoka University

Purpose : (1) Study of the processes leading to the formation of quasiperiodic relief on crystal vicinal surfaces under the layer-by-layer growth from the vapour. (2) Participation in the scientific meetings at Research Institute of Electronics, Shizuoka University during the period of stay. (3) Discussion of the research results, preparation of the publications and development of the plans of the future research.

Name of receiver : Prof. Toru Aoki

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