REPORT

by Associate Professor Daniela Bogdanova Karashanova, PhD

Institute of Optical Materials and Technologies "Acad. Jordan Malinowski",
Bulgarian Academy of Sciences

on the materials submitted for participation in the contest for filling the academic position "Professor", in the professional field 4.2 Chemical Sciences (Physical Chemistry) announced at the Institute of Physical Chemistry (IPC) - BAS for the needs of the Laboratory "Electron microscopy and microanalysis".

1. General presentation

This Report was prepared in relation with the order № 57-РД-09 dated 25.06.2020 of the Director of the Institute of Physical Chemistry – BAS where I was mentioned as a member of the scientific jury of the contest for occupation of the academic position "Professor" .

The only candidate applying in the contest, announced in the State Gazette, issue 20 dated 10.03.2020 is Associate Professor Dr. Bogdan Stavrev Rangelov from the Institute of Physical Chemistry.

2. Biographical remarks

Associate Professor Dr. Bogdan Rangelov has completed his higher education with a master's degree in physics at the Faculty of Physics of Sofia University "St. Kliment Ohridski "in 1995 and he was appointed to the position of "physicist" at the Institute of Physical Chemistry of BAS, where he defended his PhD thesis in "Physical Chemistry" in 2009 on the topic "Instability of vicinal crystal surfaces - grouping of steps". Passing successively through the various stages of his career development, in 2011 he was elected as Associate Professor in the Institute.

In his scientific career Dr. Rangelov completed a 4-year specialization in Germany - Friedrich Alexander University, Nuremberg/Erlangen, from 2000 to 2004, two specializations at the Interdisciplinary Center for Nanoscience in Marseille, France - in 2007 and 3 months in 2018 and a two-week specialization at the Institute of Semiconductor Physics, SO-RAS, Novosibirsk, Russia in 2010.

The topics on which Dr. Rangelov works during his specializations are related to the processes and phenomena occurring on crystal surfaces - molecular surface reactions and catalytic properties of crystal surfaces Pt (111) and Fe (100), spiral growth on crystal surface Si (111), waves of density of steps, directed diffusion of atomic clusters under the influence of external force, epitaxial layered growth on crystal surface Si (111). They are among the most current topics of modern materials science, sensorics and catalysis and are reflected in the topics that Dr. Rangelov develops in IPC, as well as in his publication activities. The experimental and analytical methods with which he became acquainted and worked with during his specializations are among the most modern and up-to-date in the field of surface science: reflection electron microscopy (REM), low-energy electron microscopy (LEEM), High resolution electron energy loss spectroscopy (HREELS) and of course the precise high vacuum technique required in this type of research. The experience and knowledge gained by Dr. Rangelov during his stay in foreign research centers, as well as his constant pursuit of new knowledge and skills, undoubtedly affect the quality of research he conducts and contributes

to its formation as one of the leading specialists in the field of phase formation, crystal growth, surface physical chemistry and electron microscopy.

In this regard, he received in 2008 the award "Acad. R. Kaishev" from the Scientific Assembly of IPC for scientific achievements in the field of physical chemistry. He was elected as a representative of Bulgaria in the European Network on Crystal Growth and a member of its Executive Board for the period 2015 - 2021. He has been elected as a head of the laboratory of electron microscopy and microanalysis of IPC-BAS since 2010.

3. Scientific research activity

The results of the research activity of Assoc. Prof. Dr. Bogdan Rangelov have been developed within 11 funded national projects and one on bilateral cooperation with France, as well as 2 EBR projects with Russia and Greece. They are disseminated in 41 scientific publications, in 11 of which Dr. Rangelov is the first author and one patent. All publications have an impact rank from the Scopus database. Some of them are in the renowned in the field of crystal growth and physical chemistry of surfaces Physical Review Letters (8.312 / 2013, 9.199 / 2019), Journal of Crystal Growth (1.632 / 2019), Materials Letters (3.019 / 2018, 3.20 / 2019), Surface Science (1.86 / 2009, 1.466 / 2019).

Dr. Rangelov participated in the announced competition for the academic position of "professor" with 23 publications. With them he fully covers the minimum requirements for holding this academic position, reflected in the Act for development of the academic staff in the Republic of Bulgaria and the Regulations for its implementation, as well as the regulations of IPC-BAS and even significantly exceeds them in most of the indicators.

In thematic terms, the research activity of Associate Professor Rangelov can be divided into the following 2 major areas, as he himself formulated them in the reference to the author's contributions:

I. Electron microscopic studies of phase formation processes in condensed matter
II. Simulation and theoretical studies of phase formation processes in condensed matter

The first subject area includes extensive experimental studies of two-dimensional nucleation and crystal growth (multilayer island and spiral) on vicinal crystal surface Si (111), determining its instability - waves of steps' density and critical width of terraces. This topic includes also electron microscopy studies of the processes of phase formation and characterization of glass and glass-crystal materials, soft condensed matter, thin films and catalysts.

The main contribution of the candidate is to obtain for the first time images of monatomic spirals (with a step height of one lattice parameter) of growth / evaporation on a vicinal crystal surface Si (111) by means of reflective electron microscopy with slight distortion of the image (LODREM). It is of great importance to establish the specific experimental conditions when conducting homoepitaxy experiments on a vicinal Si crystal surface (111), which subsequently made it possible to determine important characteristics such as the critical width of the terrace, transition temperature between kinetically limited and diffusion-limited mode of adatom attachment to the steps (respectively crystal growth), determination of the value of the exponent, which gives the ratio (scaling) between the critical width of the terrace and the value of the falling adatoms flow, and determination through it the size of the critical nucleus, as well as the activating energies for two-dimensional nuclei formation, the study of the so-called "transparency" of the steps.

In the research conducted on glass and glass-crystal materials, obtained by immobilization of large amounts of metallurgical waste, Dr. Rangelov's contribution consists mainly in the morphological, microstructural and analysis of the elemental and phase composition, but for obtaining significant results on these systems his participation in discussions and planning of experiments in general is very important. Dr. Rangelov participates also in the study of the structure of many other systems - adsorbed layers of oligoglycins on different types of substrates and with different concentrations, as well as of electrochemically deposited CdS layers; thin molybdenum films deposited on steel by means of a laser beam; Cu clusters in thick polyaniline films on a Pt support; carbon structures with incorporated iron, produced by a process of growth far from equilibrium - the arc between two carbon electrodes in an atmosphere of Ar and ferrocene; non-stoichiometric phases of TiO_2 as a support material for cobalt supported catalyst; titanium and chromium hard coatings obtained by magnetron sputtering and cathode sputtering. In these studies, his main contribution is aimed at establishing the structure and the existing variety of morphologies, determining the relationships between them and the varied experimental parameters, identifying and proving existing phases, etc.

The second subject area combines the results of simulation and theoretical studies of instability on vicinal crystal surfaces such as wave density of steps and Monte Carlo simulation studies of diffusion processes on vicinal crystal surfaces and it is related to the experimental studies mentioned in the formulated first subject area. In some cases the simulations were performed for verification and comparison with the experimentally-observed phenomena, while in others - the results of the numerical experiments initiated the realization of real ones.

In this regard, the effect of grouping of the steps was studied using a non-stationary Burton-Cabrera-Frank model. The influence of the electromigration force and the transparency of the steps on this instability are followed. In the case of transition from growth by movement of the steps to two-dimensional nucleation, the critical width of the terrace of the vicinal crystal surface for a fixed temperature was determined and the influence of the transparency of the steps was also established.

Monte Carlo simulation studies of the thermal stability of metal nanochains and particles with anisotropic interactions and diffusion-controlled growth in a system with two types of particles could also be included in this area.

The main contributions in this field are the theoretical and simulation results for determining the energy barrier for embedding an adatom in the "lower" step of the terrace (Ehrlich-Schöbel barrier). Theoretically/by simulations is predicted a new type of instability during the crystal growth, the so-called waves of steps density (proven and experimentally by Dr. Rangelov and co-authors) in formed pyramidal structures, the morphology of which is studied depending on the balance of the flows of adatoms that "jump" the steps in the "up" or "down" direction. Processes of diffusion of adatoms and atomic clusters on vicinal crystal surfaces and the influence of step transparency are studied, and a relatively simple model is proposed, revealing the relationship between the temperature, step roughness, applied external force and their relation to the step transparency phenomenon.

With regard to Monte Carlo simulations of the thermal stability of metal chains - two cases are presented - free-standing one-dimensional monatomic chains and two-dimensional (flat) homoepitaxial chains on the surface fcc (111). In the first case, the loss of stability was observed, starting with the appearance of vacations, which did not recover and eventually led to the appearance of holes in the chain and its successive disintegration into individual clusters.

It is determined that at a given temperature, the decrease in the strength of the interaction between the atoms of the chain is a stabilizing factor. Regarding the two-dimensional chains - the mechanism of their breaking, only under the action of thermal fluctuations, has been studied and their dependence of the stability on the number of chains in the two-dimensional strip has been established.

The presented papers also consider an extended model of diffusion-controlled aggregation of two types of particles and simulation studies, the object of which is "soft" condensed matter, which presents the interactions between model molecular complexes that are not spatially symmetric, but are directed (so-called patchy particles model).

4. Educational and pedagogical activity

To this category of activities of the candidate is presented the co-supervisor of a successfully defended PhD student.

I would like to note here that over the years Dr. Rangelov has participated many times in the Spring Seminars for PhD students and young scientists "Interdisciplinary Chemistry" organized by IOMT and has enthusiastically shared his knowledge and experience with young people. In the conducted by the Bulgarian Crystallographic Society in 2019 School of Electron Microscopy, he was one of the main lecturers and with his expertise and original presentation of the problems of electron microscopy and the dynamics of vicinal surfaces, he won the attention of participants and contributed to the success of this event.

CONCLUSION

Presented by the candidate in the contest **Assoc. Prof. Dr. Bogdan Stavrev Rangelov** documents and materials fully comply with the Act for development of academic staff in the Republic of Bulgaria, the rules for its implementation and the respective regulations of BAS and IPC-BAS, as well as on the topic of the announced contest for the occupation of Academic position "Professor". They are proof that Dr. Rangelov is an experienced scientist with a substantial contribution to the contemporary physical chemistry and surface science and electron microscopy analysis.

I am fully convinced and **I give a positive assessment** of the works and activities presented in the contest and I strongly recommend to the honorable Members of the Scientific Jury to propose to the Scientific Council of IPC – BAS Assoc. Prof. Bogdan Stavrev Rangelov to be elected to the academic position "Professor" in IPC-BAS in the professional field 4.2. Chemical Sciences (Physical Chemistry).

22.08.2020

Изготвил становището: .....

доц. д-р Даниела Карашанова