Stochastic formalism for nucleation under unsteady conditions
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Kinetics of nucleation are relatively well understood under steady-state conditions, the main problem still unsolved being the large uncertainties introduced by the stochastic nature of nucleation. To tackle this problem, a probabilistic formulation for nucleation kinetics is required instead of the deterministic formulations currently available. Some approaches in this direction have been presented mainly related to the derivation of kinetic information from experimental data [1], but a general formalism for stochastic nucleation is still incomplete at a general level.

A Langevin-type stochastic differential equation (LT-SDE) is proposed to model the fluctuating behavior of the cluster radius in the spherical shape approximation. Indeed, an analytical solution for the probability density function of induction time is obtained not only for steady but also unsteady work of cluster formation. The latter condition allows for the study of time-dependent (supersaturation, pressure, temperature, etc.) nucleation processes from a stochastic point of view.

Crystalization under unsteady conditions are getting very important in mainstream fields like protein crystal growth, where the small volumes involved and the wide metastable area in the phase diagram imposes the use of large supersaturation values induced by diffusion of the precipitant. In such conditions, the stochastic effects in nucleation are largely controlled by unsteady kinetics and can be responsible for the selection of the supersaturation at which nucleation happen (which is central for the quality of the crystals obtained) and, more importantly, the kinetic selection of polymorph.

Keywords: stochastic, nucleation, crystallization

Nucleation and growth of crystals within the frames of the quataron concept
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The problem of crystals nucleation has come into scientific use in XIX century as a problem of the origin of a new phase in the course of phase transition. More or less finished theory has been formed by the beginning of XX century. According to the classical molecular-kinetic theory of phase-formation, the nucleus of a new phase is formed as a result of consecutive joining of atoms to each other. With that, that grouping of atoms or molecules which has reached such sizes that can exist in equilibrium in the environment is called a critical nucleus. In principle, realization of these two extreme variants does not contradict the general laws of physics and chemistry. The majority of modern models of crystals growth are built within the frames of these concepts. However every year collects more and more experimental data obtained, first of all, on the basis of direct researches of the structure of crystal-forming media by spectroscopic methods and observations over growth of crystals by means of atomic-force microscopy, testifying to more extensive character of crystal-forming and to existence of differently organized atom-molecular groupings in crystal-forming media. In this connection the idea on building units as particles of larger, than separate atoms or molecules, but not crystal particles is discussed and finds more and more proofs. The ideas on the multi-path and combined character of growth of crystals become dominating. As to our quatanor concept, the mechanisms of crystals growth lying in its basis is trivial and simple. Quatrons, appearing on a growing surface of a crystal, either break up to separate atoms (further - atomic growth) or form two-dimensional nuclei (layer-by-layer growth). In rare cases they can form fractal structures on the surface (fractal growth) or inhibit growth. On their fundamental properties quatrons appeared to be ideal structures as building units. Among the advantages of the quatanor concept is that it only operates with nonequilibrium structural units at description of crystals growth, which, in turn, also takes place only in nonequilibrium conditions. The basic laws of formation and growth of crystals find explanation within the frames of the quatanor concept.

Keywords: crystallization, nucleation, cluster.
crystal occurs mainly due to the expansion of elementary layers of growth. They are 8.8 Å units high, which is equivalent to parameter \( a \) of a unit cell, and give the peculiarities of the specific structure, is also equivalent to one of the sizes of \( C_{60}H_{50}N_{20}O \) molecule.

The statistical data processing reveals considerable differences in tangential dissolution rate on the two spirals, consisting of nine and four screw dislocations correspondingly. Right-screw growth layers of the left spiral join, at some distance, the left-screw steps of the right spiral, forming an even more complex source – a growth analogy of disociational Frank-Read source. To calculate the tangential rates for such source, each image was overlaid by a special grid axiffed to defined points – canals of dislocations. Then the position data of intersection points of grid meridian and the step contour were taken. Each two images required more than a thousand of coordinate readings. Then we schemed the step rate distribution for every image pair. The distribution came out to be bimodal, which required segregation of the results for the left and the right spirals. Each distribution was then approximated to the lognormal distribution, average tangential rates were determined as expectation value, and rate fluctuations were calculated as a mean-square deviation. The results show that for the left source steps the average tangential rate is two times greater than that for the right source ones throughout the whole experiment. On the whole, the tangential rate decreases towards the end of the experiment. The rate fluctuations for the steps of both groups also reveal an almost monotonous decrease. This means that the system is working towards equilibrium. The amount of substance in the solution is increasing and dissolution is going to give place to equilibrium. This brings forward an important inference: the left and the right part of the same growth source, located at a less than a micrometer distance from each other, have a different effect on the boundary layer of the solution. We have shown that the interface needs to have the horizontal concentration gradient of the substance which would provide a faster tangential rate of the left spiral at growth and a more active decrease at dissolution. The same assumption has been verified for bigger (100 mmk) hillocks.

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Keywords: AFM, crystal, growth.

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In situ observation of stress and strain evolution during surfactant-mediated growth of Ge on Si

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Interplay of surface stress and surface free energy determines the growth mode of heteroepitaxial layers. Therefore, surface morphology is sensitive to the presence of a third species on the surface, so-called surfactant. For instance, it is well known that the Stranski-Krastanow (SK) growth mode of Ge on Si can be suppressed with the surfactant. In such a surfactant-mediated epitaxy (SME), a flat Ge layer grows on Si while the surfactant floats up to the growth front and always covers the Ge surface. The stress in the Ge layer is relaxed by injection of dislocations into the Ge/Si interface.

Recently, Bi has attracted a lot of attention as a surfactant for Ge/Si(111) heteroepitaxy due to its ability to suppress Ge-Si intermixing and provide a chemical contrast between Ge and Si in a Scanning Tunneling Microscope (STM), allowing fabrication of self-organized Ge/Si(111) nanostructures on the Si surface during STM measurement. In addition, low incorporation of Bi in the Ge layer allows to remove it from the flat Ge surface even after Bi-mediated growth.

We have focused on the stress and strain evolution during the initial stages of Bi adsorption on Si(111) 7x7 and Bi-mediated growth of Ge on Si(111). The stress and strain behavior and surface morphology were observed simultaneously by using real-time measurements of the substrate curvature and Reflection High Energy Electron Diffraction (RHEED). We find a clear difference in the surface stress between the clean Si(111) 7x7 surface and the Si(111) √3x√3 surface covered with one monolayer of Bi (1 ML = 7.8x10⁴ atoms/cm²). Subsequent Ge deposition on Bi-adsorbed Si surface provides an increase in compressive surface stress accompanied by simultaneous stress and strain oscillations. The compress stress is followed by clear stress relaxation at the critical coverage of 2 bilayers (1 BL = 2 ML) due to a variety of strain relief mechanism including injected misfit dislocation and increasing surface roughness on the Ge surface.

Keywords: epitaxy, heterostructure, stress

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Hydrothermal Synthesis of New Er₅Ni₃Zn₀.5O Nanomaterials and Their Physical Properties

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Zinc oxide (ZnO) is a wide-gap semiconductor, which is transparent from the visible to infrared regions and is resistant to reductive ambient. Because of these properties, it is expected to be applicable as a material for transparent electrode and window layers of solar cells. Among the different methods of synthesis of ZnO nanostructures, the hydrothermal method is attractive for its simplicity and environment friendly conditions. In this research, New Er₅Ni₃Zn₀.5O based nanomaterials were prepared by hydrothermal method. Zn(NO₃)₂.6H₂O (x<<1 mmol) and NaOH (0.6 g) were added to distilled water (60 mL), and stirred well for 20 min at room temperature. Afterwards, Ni(NO₃)₂.6H₂O and Er₂O₃ with various stoichiometric ratio were added, and the mixture was transferred to a 100 mL Teflon lined autoclave. The autoclave was sealed, maintained at 180 °C for 48 h, and then cooled to room temperature. The white precipitate obtained was filtered and washed with ethanol and water. Powder XRD patterns indicate that the Er₅Ni₃Zn₀.5O crystals (x = 0.00-0.04) are isostructural with ZnO. SEM images show that co-doping of Er³⁺ ions in the lattice of ZnO results in different nanorods and nanoparticle morphology. UV-Vis absorption and emission spectroscopy reveals mainly d-d electronic transitions of the Ni²⁺ ions in case of nanomaterials.


Keywords: hydrothermal, semiconductor, solar cells

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A Novel Three Dimensional Framework Induced by π–π Stacking of 2,2’-(alkylene-1,6-diyl)dilsoquinolinium from Q[6]-based Pseudorotaxane

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