the surface is particularly smooth [1].

[1] Vonk V., et al., *ESRF Highlights*, 2004 (2005).

Keywords: laser ablation, superconductor films, synchrotron X-ray diffraction

P.16.06.2

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Crystallization of $RAl_3(BO_3)_4$ and $R:YAl_3(BO_3)_4$ Single Crystal Layers

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Current development in miniature optical components leads to extensive study of single crystal layers because of a number additional benefits such as ability to use materials with high doping levels or to obtain high gain with modest pump powers. New crystals of solid solutions based on the $YAl_3(BO_3)_4$-$RAl_3(BO_3)_4$ (YAB-RAB) systems are promising solids for self-frequency doubling lasers [1].

In this report, our recent results on liquid-phase epitaxy (LPE) of RAB and R:YAB single crystal layers are discussed. Variations of growth rates of these layers were determined, in order to control crystal growth mechanism. Relations between the growth rate V and relative supersaturation β were found. It is also shown that primarily volume and surface processes occur simultaneously although evidence is presented for kinetic limitation of the growth rate on the later stage.

Besides, growth spirals epilayers frequently exhibit irregularities such as cusps and corrugations, but flat areas may also present on the surface. Micromorphological features as well as growth kinetics greatly depend on the substrate perfection.

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[1] Dorozhkin L.M., Kuratev I.I., Leonyuk N.I., Timchenko T.I., Shestakov A.V., *Sov. Tech. Phys. Lett.*, 1981, **7**, 555.

Keywords: liquid epitaxy, epitaxial layers, kinetics and mechanism of crystal growth

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RHEED Observation of c-GaN on 3C-SiC/Si(001) Template Grown by RF-MBE

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Cubic gallium nitiride, c-GaN, can be used to grow on a cubic substrate with a suitable latice constant for lattice matching. Cubic silicon carbide, 3C-SiC, which was formed by the carbonation of Si surface using a C_2H_2 jet nozzle[1], was used as a substrate for the epitaxial growth of c-GaN. The grown c-GaN layer was analyzed by reflection high energy electron diffraction (RHEED), electron microscopic techniques, and X-ray diffraction (XRD) techniques.

For the growth of the GaN layer, a specially designed RF-ECR type N radical source of 13.56 MHz was used to efficiently eliminate N ions and electrons from the surface [2]. The initial carbonization and initial growth of a LT buffer layer of c-GaN were monitored using RHEED during growth. The GaN was found to have the (2x2) surface structure. A GaN layer 1.5-mm thick grew epitaxially on the (001) face. The relative intensity ratio between cubic (002) and hexagonal(h) (10-11) XRD peaks from the GaN was 0.95:0.05.

[1] Kikuchi T., et. al, *J. Crystal Growth*, 2005, **275**, *in press*. [2] Ohachi T., et. al., *J. Crystal Growth*, 2005, **275**, *in press*.

Keywords: epitaxial layers of c-GaN, in situ observations by RHEED, RF-MBE

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Photoluminescence Study of Selenium Doped GaSb Layers Grown by Liquid Phase Epitaxy

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We analyzed the photoluminescence spectra of selenium-doped GaSb grown by liquid phase epitaxy at several temperatures from 10-160 K. The growth was performed using the same solution on GaSb substrates at 450 °C. The obtained layers showed only a small variation of carrier concentration. Photoluminescence measurements at 10 K showed a dominant transition near 777 meV associated to the residual acceptor. The dominant residual acceptor has been attributed to the native defects caused by antimony deficiency, usually due to the Ga antisite or Ga antisite defect in combination with the Ga vacancy. Also at this temperature, there are observed several bands associated to the presence of selenium shallow donors. As the measurement temperature increases, the photoluminescence band associated to the GaSb energy bandgap dominates the spectrum and its temperature dependence agrees with those for the case of tellurium and sulphur doped GaSb.

Keywords: GaSb, photoluminescence, liquid phase epitaxy

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Substitutional and Interstitial Inclusions of Mn Additivies onto the KDP Lattice

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In this work, pure and Mn^{3+} doped potassium di-hydrogen phosphate (KDP and KDP:Mn) were studied through Rutherford back-scattering (RBS), Rietveld refinement (RR) and X-ray n-beam diffraction (nBD). RBS results allows the determination of KDP:Mn stoichometric formulae as $KH_2PO_{3.8}Mn_{0.4}$ while, from the RR results, it was possible to determine that the Mn^{3+} atoms are substitutional to the K ones. The lattice parameters were determined for both pure and KDP:Mn by using RR and nBD and, besides agreeing very well, they indicate the better accuracy of the results from nBD. This fact comes from the high sensitivity of the nBD technique in determine micro-crystallographic variation. According to the lattice parameter results, all values for KDP:Mn are smaller than those for KDP. Those results are also compared with a previous one, were it was determined that Mn^{3+} in concentration of 2-5 x 10^{-4} mol are occupying interstitial sites [1] and located 0.66 from (200) plane and 0.21 from (112) plane [2]. Rietveld refinement was performed from X-ray high-accuracy single crystal measurement and the nBD measurements were carried out at beam line XRD1 of the Brazilian Synchrotron Light Laboratory. All samples were grown at the same pH of 1.5.

[1] Lai X., Roberts K. J., Avanci L. H., Cardoso L. P., Sasaki J. M., *J. Appl. Cryst.*, 2003, **36**, 1230-1235. [2] Lai X., Roberts K. J., Sasaki J. M., Cardoso L. P., Bedzyk M., Lyman P. F., 2005, *in preparation*.

Keywords: X-ray difraction techniques, inclusion phenomena, Rietveld structure analysis

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New Routes in Carbon Nanotube Synthesis by Means of a Modified Hot Filament Chemical Vapor Deposition Technique

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Our Hot Filament Chemical Vapor Deposition (HFCVD) apparatus, modified by the introduction of a powder flowing system, allows the use of different kinds of solid powders as reactants. By the use of $Fe(NO_3)_3$ in acetone as a catalyst, and carbon nanoparticles as reactants, we successfully synthesized Single Wall Carbon Nanotubes (SWNTs). We proved able to control orientation of the deposit as well as the area of growth [1]. By slightly varying experimental conditions, we obtained a nanocrystalline diamond coating on SWNT wall [2]. The use of diesel soot as SWNT precursor has been investigated, too: highly oriented growth of tubular structures through catalysed reaction occurs all over the substrate with abundance of coiled, intriguing structures. Commercial graphite with powders' size in the micron range, in the same experimental conditions, lead to Multi Wall Carbon Nanotube rich deposits. Selected area growth of nanotubes can be achieved by means of catalyst dispersions on Si/SiO_2 patterned substrates or from selectively sputtering metallic iron

[1] Orlanducci S., Sessa V., Terranova M. L., Rossi M., Manno D., *Chem. Phys. Lett.*, 2003, **367**, 109S. [2] Terranova M.L., Orlanducci S., A.Fiori, Tamburri E., Sessa V., Rossi M., Barnard A.S., *Chem Mater.*, *submitted*.

Keywords: nanotubes, nanostructures, chemical vapor deposition

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"Latent" Phase Clusters (Kvatarons) as Growth Units

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In a number of our works (Askhabov, 1998-2004) we have described a set of ideas and principles dealing with structural organization of substance in the nanorange. This ideas have been collectively referred to as "kvataron concept". Central in this new concept is the idea that there are specific nanosize clusters, which we call kvatarons, arising under non-equilibrium conditions. Physically, kvatarons are pre-crystallization clusters of the transient ("latent") phase. It has been found that clusters more than ~1.2 nm in size can become potential centers of crystallization. Only such clusters contain a minimal number of atoms necessary for crystal nucleation. At the same time, crystals grow by smaller clusters (kvatarons), which are transformed to "two-dimensional" nuclei already on the growing crystal surface. We have proposed a new theory of crystal growth, were kvatarons are the basic growth units. Kvatarons are ideal as growth units. Chemical composition of kvatarons is the same as that of crystals. Topologically kvatarons are close to structural modules of crystals. Variability of the structure allows kvatarons to join any crystal surface. A growing crystal itself actively influence on kvataron crystallization on the crystal. The kvataron model accounts for all fundamental aspects of crystal growth: growth kinetics, surface evolution, defects formation, impurity entrapment, etc.

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Keywords: nucleation and crystal growth mechanism, clusters, kvatarons

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Numerical Modeling of Interaction of Particles with Solidifying Crystals

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The thermal fields for the movement of a solidification interface towards a spherical particle was dynamically modeled for studying the deformation of the interface in relation with different thermal properties of the particle with the matrix solid-liquid. Finite element methods were employed in an axi-symmetric model of the system. Both particle and matrix were considered of similar densities and heat capacity. The convective force in the liquid phase was not considered. The results show that a concave interface is found when the particle has a larger thermal conductivity than the matrix, and a convex interface is found in the opposite case.

In addition, the drag force on a particle being pushed by a crystal was calculated with a fluid flow model. The force was calculated for different pushing configurations and the results compared with the values given by the modified Stokes equation [1]; which show that the model value are slightly larger than those the calculated with the equation. This difference predict an equilibrium separation for pushing lower than the computed by modified Stokes expression when a Lifshitz-Van der Waals model for the repulsion force [2] is used.

[1] Uhlmann M.A., Chalmers B., Jackson K.A. *J. Appl. Phys*., 1964, **35**, 2986. [2] Dzyaloshinskii E., Lifshitz E.M., Pitaeskii L.P., *Soviet Physics*, 1961, **73**, 153-176.

Keywords: computer simulation of solidification, melt growth, pushing

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Crystal Growth and Morphology Prediction of Two Quinacridone Polymorphs

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Quinacridone – a widely used organic pigment – is known to have three polymorphs. Two of them, the beta-polymorph and the gamma-polymorph, grow as very thin platelets.

Vapour growth starting from both polymorphs was performed by vacuum sublimation in a specially constructed furnace. During characterization of the polymorphic phases by DSC recrystallization was observed. This led to the formation of beta-crystals. The new polymorph was formed via the vapour phase.

To explain the observed morphology of the crystals computer simulation of crystal growth was performed. Both the attachment energy model and kinetic Monte Carlo simulations were used to predict the crystal morphology starting from the crystal structure. The crystal structure of the gamma-polymorph is known from the Cambridge Structural Database and the crystal structure of the beta-polymorph was predicted using the Polymorph Predictor of Accelrys.

The attachment energy model based on the Hartman Perdok theory fails to predict the large aspect ratio of the platelet morphology for the polymorphs. The kinetic Monte Carlo simulations use the actual crystal structure and growth mechanism; they predict the morphology of both polymorphs successfully.

Keywords: polymorphism, crystal morphology, crystal growth computer modelling

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MONTY: An Algorithm for Predicting Growth Rates for any Crystal Structure in any Orientation

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A crystal growth simulation program, based on the Monte Carlo algorithm, is presented. The experimental crystal structure is input for the algorithm. It is modeled by a set of molecular interactions, which are obtained from molecular mechanics calculations. The mother phase is parameterized by its bulk thermodynamic properties. As a result, besides the growth rate, the microscopic surface structure can be studied under various growth conditions. [1].

Two examples are presented. The program was used to simulate the growth of two polymorphs of aspartame; the extreme aspect ratio of the experimental needle crystals is well-predicted [2]. The second example involves naphthalene. There it is shown, using the spiral growth option in the algorithm, that it is impossible to grow crystals of naphthalene at moderate supersaturations without the presence of screw dislocations. This is supported by using AFM [3].