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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

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**Keywords: nanotubes, nanostructures, chemical vapor deposition**

**P.16.10.1**

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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.

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**Keywords: computer simulation of solidification, melt growth, pushing**

**P.16.10.3**

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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**

**P.16.10.4**

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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].