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X-ray Line Profile Analysis of CeO_2 Nanoparticles
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Microstrain and crystallite size characteristics of nanomaterials are important as they define the mechanical, optical and electronic properties of the specimen. By characterising these parameters in a test-bed material such as cerium oxide (CeO_2) nanoparticles, complex physical models can be developed to fit experimental X-ray diffraction data. This understanding is crucial for creating complex polytypic structures that can be used to develop more advanced materials and further the already growing nanotechnology industry.

In this paper the X-ray line profile analysis is used to quantify the dislocations and size distribution of CeO_2 nanoparticle samples. The analysis quantifies the density of dislocations, while the crystallite size properties are quantified in terms of size distribution and modal properties of the CeO_2 specimens.

The CeO_2 nanoparticle specimens studied here are bimodal admixes that comprise varying proportions of ~30nm and ~5nm nanoparticles. X-ray line profile analysis is used to quantify the dislocation and size distribution for these samples. These results are compared with experimental TEM measurements of the samples.
Keywords: line-profiles, nanoparticles, dislocations

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Application of Molecular Modelling to Study Nucleation, Impurity Segregation, Solvent Adsorption and Polymorphic Transformation
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Calculating the correct lattice energies is the basis for modelling molecular crystals. The semi-empirical method within the atom-atom formalism has been successfully applied to many organic systems before. Lattice energy of polar crystals like γ-glycine where the electrostatic component plays a vital role could not be evaluated successfully by this method. A combined approach using both semi-empirical and quantum mechanical methods within a periodic formalism has been adopted for successful calculation of lattice energy. Subsequent to this, prediction of crystal shape, additive effect on the host lattice, solvent effect on the surface energies of (hkl) habit faces and energetic stability of polymorphic modifications of the crystal have been modelled. The additive effect on the shape of the host crystal has been studied using semi-empirical method. Segregation coefficient determines the impurity incorporation at the host lattice. Differential binding energy which is proportional to the segregation coefficient can be calculated from the slice and lattice energies. The predicted crystal shapes enable the construction of polyhedral molecular clusters via overlaying the morphological simulation model with the crystal structure. The relationship between the energetic stability and cluster size in polymorphic system, l-glutamic acid has been studied. Further, an attempt has been made via modelling to calculate surface energy values to allow surface dependent (or anisotropic) interfacial tensions to be calculated within the formalism of classical homogeneous nucleation theory.
Keywords: morphology, polyhedral clusters, binding energy

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Development of Crystallographic Textures in Diamond Films
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Polycrystalline thin films develop a crystallographic texture that is dependent on the environmental conditions during the deposition process. In these experiments, analysis of the preferred orientation plays an important role in understanding the relation between the growth process at the surface of the sample and its final microstructure. Special attention has to be paid to the role of impurities since they are known to disturb the growth process. Their presence can lead to different morphological structures and to different materials properties.

It has been demonstrated in literature that the presence of nitrogen in the gas phase during deposition of diamond thin films by chemical vapour deposition techniques has a large influence on the morphology of the final layer. In the present study, a detailed analysis is given of the development of texture in diamond thin films during the deposition process from the gas phase and the role of nitrogen therein. The preferred orientation of the films were studied using X-ray diffraction as a function of the content of nitrogen deliberately added to the gas phase during the deposition process. The results have been compared with the morphological changes of the sample surfaces. A model has been developed that describes the role of nitrogen during incorporation at the growing diamond {111} and {100} faces.
Keywords: diamond, microdiffraction, preferred orientation

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New Tools for Microstructure Analyses of Polycrystalline Materials using an X-ray Area Detector
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X-ray diffractometers equipped with an area detector are very powerful tool for polycrystalline material characterization. From the 2D diffraction patterns of a polycrystalline samples, collected using an adequate exploration procedure, important microstructure information (grain crystal size and crystallographic texture) can be extracted. Here, we present some hardware and software tools for automatic microstructure analyses. For instance, XtalSizer automatically determines a set of parameters from a single 2D diffraction pattern that characterize the sample crystal size in the micrometric range. Real crystal sizes can be determined after proper calibration with standards samples with known sizes. This technique is independent of the aggregation state of crystals in the sample; It can be used in powder samples as well as in densely packed samples (i.e., ceramics). Also, the range of size determined (tens to hundreds of microns) are complementary to crystallite size determined from the broadening of Bragg peaks (0.1 micron and below) increasing the potential of X-ray diffraction techniques to characterise polycrystalline materials. We have also developed another software tool, XTexture, that calculate and plots the pole figures from a set of 2D diffraction patterns. This software tools allow fast determination of microstructural information that using other traditional techniques (i.e, optical microscopy, X-ray texture diffractometer) would be very tedious to acquire.
Keywords: CCD area detector, crystallographic texture, grain size

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Local Elastic Measurement in Nanostructured Materials via Atomic Force Acoustic Microscopy Technique
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Atomic Force Acoustic Microscopy (AFAM) [1] is an emerging AFM based dynamical technique that allows one to acquire simultaneously images reflecting samples morphological and mechanical characteristics with nanometrical resolution, and to quantitatively evaluate sample local Young modulus. The AFM system must be equipped with a suitable piezoelectric transducer exciting longitudinal oscillations at ultrasonic frequencies in the sample under investigation. Measured resonance frequencies of