

100ps resolution by this method.

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Indexing algorithm for powder diffraction pattern using topograph

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Indexing of powder diffraction patterns is considered as the most difficult part among the procedures of ab-initio powder structure determination. Recently, we devised a new indexing algorithm that can search rapidly and thoroughly for the possible solutions. Topograph is a connected tree in the graph theory, which is a collection of relation formula given by $Q(h_1+h_2) + Q(h_1-h_2) = 2 * (Q(h_1) + Q(h_2))$. Although this formula is already known as Ito's equation and used in Ito's algorithm, it takes a more powerful role in our method as a basis of the equations among the Q-values of the peaks. Extinction rule is troublesome, but it is somehow obtained without information on the symmetry, in the process to construct the topograph. The algorithm is proved to work completely at least for lattices of dimension 2. For the case of dimension 3, some uncertain part still remains. The algorithm works without any assumption on Bravais lattice. It is efficient even if there is a false peak in the powder diffraction pattern or the material is not a single phase. The detail of the method and some results are introduced.

Keywords: powder indexing, *ab-initio* powder structure determination, computer algorithms

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Structural characterization and developing a suitable SAXS model of diblock(DEAEMAn-DMAEMAm) polymers

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Small Angle X-ray Scattering (SAXS) is a powerful method to investigate nano-aggregations formed by self-assembly of block

copolymers in melt, solution or crystal state [1]. In this study, theoretical scattering models such as spherical core-shell and ellipsoidal core shell micelle models were described and discussed after the performed SAXS measurements at NSRRRC-Taiwan beside the determination of the morphologies. The studied di-block copolymers [2-(diethylamino)ethyl methacrylate (DEAEMAn)] · [2-(dimethylamino)ethyl methacrylate (DMAEMAm)] had been synthesized by Vural Bütün as a part of a serial research on pH dependent-water soluble block copolymers [2-3]. Our previous studies have been showed that micellar aggregations are expected due to hydrophobic and polyelectrolyte ends of polymeric units [4]. Two samples which have 23576 and 12177 g/mol molecular weights were prepared for SAXS measurements. Model-independent approximations with Guinier, Porod and Kratky plots together with the results of static and dynamic light scattering (SLS and DLS) are used to extract morphology characteristics, on which basis, a suitable model shape is chosen to fit the SAXS profiles. Beside of these investigations, a semi-empirical calculation method (PM3 [5]) was also used to examine crosslink effect of free polymeric units. So, electron densities in the layered thicknesses were also predicted before construction of the models. At the end of the study, the details related with mathematical and physical explanation for the models are also described in this presentation.

Keywords: DEA, DMA, Core-shell, SAXS, DLS, SLS, PM3, Nano structures

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High-pressure phase transformations in aragonite, strontianite and witherite

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We have studied structural phase transformation in aragonite CaCO₃ and related isostructural compounds strontianite SrCO₃ and witherite BaCO₃ at high pressure by performing first principle calculations. The following phase transition sequence *Pmmn* - *Pmnc* - *C222₁* have been found for all three compounds. Furthermore, CaCO₃ and SrCO₃ undergo a phase transition from *C222₁* to *Pmmn* modified-aragonite phase at very high pressure as a result of carbon sp² to sp³ transition. Thus the structural trends of these compounds are determined by both the cation size and the chemistry of CO₃ group. The formation of sp³ hybridized bonds is driven by the intrinsic property of the carbon atom to form tetrahedrally covalent bonds at high pressure and explains the stability of MgCO₃ and CaCO₃ at the Earth's lower mantle pressure conditions. The presence of sp³ hybridized carbon may serve as a criterion for new possible high-pressure phases of carbon bearing minerals.

Keywords: *ab-initio* calculations, high-pressure phase transformations, carbonates

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Crystal structures of moderately complex organic molecules are predictable

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