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ON THE INFLUENCE OF THERMAL MOTION ON THE CRYSTAL STRUCTURES AND POLYMORPHISM OF EVEN n-ALKANES

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Discrepancies between the crystal structures of short n-alkanes as obtained from experiment and as obtained from molecular mechanics turned out to worsen at longer chain lengths. The same holds for the relative stabilities of the two experimentally observed polymorphs. In this talk it is argued that the discrepancies are due to thermal effects, and that the triclinic polymorph is the most stable polymorph for all chain lengths at 0 K. A phase transition is predicted that yet has to be found experimentally. Current force fields cannot reproduce the experimental observations without explicit introduction of temperature by means of molecular dynamics.

Keywords: THERMAL MOTION n-ALKANES MOLECULAR MODELLING

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HARD X-RAY TOMOGRAPHY WITH A MICROFOCUS SOURCE AND INCLUDING PHASE CONTRAST

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A description of high-resolution hard X-ray tomography results obtained using a charge-coupled device (CCD) detector and a laboratory-based microfocus source for various objects will be presented. In addition to absorption contrast, such a source provides the necessary spatial coherence (for appropriate source-to-object distance R_1) to achieve significant phase-contrast contributions in the individual two-dimensional intensity distributions (image frames), a high degree of chromatic coherence not being required. Relatively large object-to-image distances (R_2) are employed to allow wave interference (Fresnel diffraction) effects to occur and result in contrast formation at the image plane. The geometry used provides for edge enhancement of certain object features, inherent magnification, improved signal-to-noise and reduced contribution from scatter. The salient features and advantages of this imaging modality will be demonstrated via systematic variation of particular experimental parameters such as source operating voltage, source size, R_1, R_2, number of image frames and detector resolution, and via theoretical (Kirchhoff formulation) image simulations. A detailed discussion of the processing of such X-ray intensity data sets will also be given.

Keywords: TOMOGRAPHY MICROFOCUS SOURCE PHASE CONTRAST

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PHASE-CONTRAST MICROTOMOGRAPHY USING COHERENT SYNCHROTRON RADIATION

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The outstanding characteristics of third generation synchrotron radiation sources enabled the improvement of existing x-ray imaging techniques based on absorption, but also the development of new approaches based on alternative contrast mechanisms such as the optical phase. State of the art absorption tomography provides the three-dimensional mapping of the linear attenuation coefficient in the bulk of millimeter-sized samples with a spatial resolution in the order of 1 micrometer. It was applied to obtain microstructural and/or quantitative information on a large variety of materials (metal alloys, porous materials such as snow, biological samples such as wood or bone). However, in many cases conventional absorption contrast fails and the improved sensitivity of phase imaging is highly beneficial. The coherence of modern synchrotron beams makes a trivial form of phase-contrast imaging based on propagation possible. The propagation technique can be used either in a qualitative way, mainly useful for edge-detection, or in a quantitative way, involving numerical retrieval of the phase from images recorded at different distances (typically three or four) from the sample. The combination with tomography allows to reconstruct the electron density in the sample with micrometer resolution. This combined approach is called holotomography. It was applied to several problems in materials and life sciences when it is crucial to enhance the sensitivity or reduce the dose compared to absorption tomography. The figure shows a 3D rendering of the liquid phase in an al/si alloy (collaboration with l. Salvo, GPM2, Grenoble). The dose reduction and increased sensitivity in phase imaging are crucial for imaging thick biological samples in their natural, wet environment.

Keywords: MICROTOMOGRAPHY PHASE RETRIEVAL SYNCHROTRON RADIATION

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MAGNIFIED HARD X-RAY IMAGING AND TOMOGRAPHY IN ABSORPTION AND PHASE CONTRAST

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Parabolic refractive X-ray lenses (PRXLs) are high quality imaging optics for hard X-rays that are particularly suited for the use as an objective lens in a hard X-ray full field microscope. With aluminium lenses, a resolution of about 300 nm was achieved in a field of view of about 300 μm. Using more transparent lens materials, such as beryllium, the resolution is expected to be improved down to 50 nm in a field of view of about 1 mm. The large depth of field (several mm) of the microscope yields sharp projection images for most samples. This allows to combine magnified imaging with tomographic techniques. Using a microprocessor as a test sample, the resolution of magnified tomographic imaging is investigated. A three-dimensional resolution of about 300 nm was observed with aluminium as lens material. By controlling the degree of coherence of the radiation incident on the sample, the microscope can be operated in both absorption and phase contrast. Recording a series of defocused X-ray micrographs allows one to reconstruct the complex transmission function of the object.

Keywords: HARD X-RAY MICROSCOPE REFRACTIVE X-RAY LENSES CONTRAST FORMATION