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TOWARDS THE AUTOMATION OF PROTEIN CRYSTALLOGRAPHY ON THE SRS

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A project is currently underway to automate the protein crystallography beamlines on the Synchrotron Radiation Source (SRS) at Daresbury Laboratory. Included in this project is the development of an automatic sample changer to allow remote mounting and dismounting of frozen protein crystals and the upgrade of all of the experimental equipment on the station in order that all required movements can be controlled from outside of the experimental hutch.

Currently development work, concentrated on the sample changer, is being carried out off-line and on Station 7.2, a protein crystallography development station. Once satisfactory operation has been achieved the equipment will be transferred to Station 14.2 and commissioned for user operation.

Once Station 14.2 is successfully commissioned as a fully automated facility then further expansion to encompass other protein crystallography stations on the SRS will be considered.

Keywords: SYNCHROTRON RADIATION INSTRUMENTATION BEAMLINE AUTOMATION ROBOTIC SAMPLE CHANGER

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DEVELOPMENT OF A VACUUM CHAMBER FOR AN CLOSED CYCLE HELIUM CRYOSTAT WITH MINIMUM BACKGROUND

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The use of closed cycle Helium cryostat in low temperature diffraction experiments has considerable advantages in comparison to open flow systems, because the running cost are low and the temperature can be held stable for a long time. In neutron diffraction these chambers are made of Aluminium or Vanadium resulting in low background, but for x-ray diffraction only Beryllium and Carbon chambers have been used. This results in high background with powder lines for X-ray diffraction. This is especially a problem when area detectors are used, because it is not possible to reduce the background with a detector collimator. To overcome this problem a vacuum chamber was construced from 0.1 mm Kapton film. This results in a very low background in comparison to a Beryllium cylinder. The use of this film without supporting material in the X-ray beem becomes possible through the construction of a two side support on a large Huber Diffractometer to span the film enough to hold atmospheric pressure. The construction has a low leak rate making it possible to measure at least 7 days at 15 K without pumping and even longer periods with pumping. It is possible to use normal or metallized film so that the crystal is even visible with this setup if needed.

Keywords: HELIUM CRYOSTAT AREA DETECTION

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THE POSSIBILITY OF ATOM CLUSTER IMAGING BY FREE ELECTRON X-RAY LASERS

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Linac based free electron lasers will produce extremely short (<100fsec) and intense hard X-ray pulses (1012ph/pulse). The unique features of this beam will allow the study of the atomic structure and the different physical and chemical processes in solids at a level not accessible today. However, to understand the experimental results one has to have a detailed picture of what happens during the burst in the sample. In several suggested applications small samples containing only 103-106 atoms are the possible candidates. In order to have a feeling about the atomic motions, we performed model calculations on the dynamics of particles of a cluster in an intense hard x-ray pulse. The parameters of the pulse were chosen to be in the range of the planned free electron lasers. The movement of the particles was followed by non- relativistic classical dynamics. The main processes: photo-absorption, Auger process, inelastic and elastic scattering of electrons were taken in to account by their respective cross sections. Here we report our findings on all carbon atom clusters. The results show that the clusters disintegrate via Coulomb explosion, similarly to small clusters in intense laser beam. However, the dynamics of the explosion is significantly different. We analyzed our data from the point of view of structure determination [1]. We found that the number of ionized particles increases faster than expected in previous studies. Therefore collection of useful data is possible in the first 10% of the pulse.

References

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Keywords: X-RAY, LASER, MOLECULAR IMAGING

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APPLICATION OF THE LDE METHOD TO A COMPOSITE CRYSTAL STRUCTURE

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The Low Density Elimination (LDE) method, which was originally developed for solving macromolecular crystal structures, has recently been applied to several quasicrystals for determining positions and shapes of occupation domains in n-dimensional unit cell (Takakura et al. 2001). In the present work, the method is applied to an incommensurate composite crystal using superspace description. The structure of $Ca_{13.6}Sr_{0.4}Cu_{23.983}O_{41.965}$ (Ohta et al. 1997) with super space group $F222(00\gamma)$ is chosen as a test structure. Calculated structure factors from the refined model are used. The density modification process is carried out in the four-dimensional unit cell. Starting from random phase sets, 4 resultant sets out of 100 trials has reasonably low phase errors. The four dimensional density maps reveal atoms as wavy strings. Although the error-free data has been used for the test, this result indicates possibility of *ab initio* structure determinations of incommensurate composite crystals by the LDE method.

Keywords: DENSITY MODIFICATION COMPOSITE CRYSTAL AB INITIO METHOD