TiO_2 (rutile modification), space group (136) $P4_2/mnm$, carried out in the vicinity of the Ti-*K* absorption edge. The influence of oxygen vacancies on the anomalous scattering signal (see e.g. [2]) has been studied on a series of 10 x 10 x 1 mm^3 single crystal wafers of different vacancy concentrations obtained by annealing at a temperature of 800°C in a vacuum of about 10^{-6} mbar for different durations. Considered reflections include the 'forbidden' 001 and allowed 111 reflection. Simulations by means of *ab-initio* modeling of the near-edge transitions and an interpretation of the far-edge resonances based on vacancy-induced static Ti displacements from high- to low-symmetry positions will be presented.

[1] V.E. Dmitrienko, E.N. Ovchinnikova: *Acta Cryst. A56* (2000) 340.
[2] V.E. Dmitrienko, K. Ishida, A. Kirfel, E.N. Ovchinnikova: *Acta Cryst. A61* (2005) 481.

Keywords: DAFS, anomalous scattering methods, resonant scattering

FA5-MS38-P10

Automated Seeding for the Optimization of Crystal Quality. Naomi Chayen[a], Lesley Haire[b] and Sahir Khurshid[a], [a]*Biomolecular Medicine, Imperial College London, UK,* [b]*National Institute for Medical Research, Mill Hill, UK*
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With the advent of structural genomics a variety of crystallization techniques have been automated and applied to high throughput, yet seeding which is the most common and successful optimization method is still being performed predominantly manually. The aim of this study was to devise simple automated seeding techniques that could be applied in a routine manner using existing robots and without the requirement of specialised tools. Two alternative protocols for automated seeding experiments are described. One involves the delivery of micro-crystals from stock to target wells using the robot dispensing tip as a seeding tool. The second harnesses an animal whisker as the seeding tool. Larger, better ordered crystals were obtained using both techniques.

Keywords: protein crystallization, automation, seeding

FA5-MS38-P11

Upside Down Protein Crystallization. Naomi Chayen[a] and Sahir Khurshid[a], [a]*Biomolecular Medicine, Imperial College London, UK*
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A technique leading to the formation of the highest ever diffracting crystals of 'Human Myosin Binding Protein C' (MyBPC) is described. This method was initially designed to facilitate the use of the microbatch method in microgravity. The crystallisation vessels currently employed for microgravity crystallisation are non-optimal with regards to cost, sample volume, size and ease of use. The utilisation of microbatch experiments is a favourable alternative in each respect: To date, the use of microbatch has not been pursued due to concerns of oil leakage. To address this issue, a novel approach is described where the microbatch plates are inverted throughout the duration of the experiment. The findings intimate the application of the microbatch method to space flight and the potential to significantly increase the output of microgravity crystallisation research. Furthermore, crystallisation in the inverted position was found to be enhanced with crystals of the target MyBPC diffracting to the best ever obtained resolution of 1.2Å. It is proposed that this can be attributed to the negation of drop contact with the crystallisation vessel enabled by this method in a manner similar to containerless crystallisation.

Keywords: protein crystallization, optimization, microbatch

FA5-MS38-P12

Electronic Carbon-Nanotube-Based Materials for Protein Crystallization. Naomi E. Chayen[a] Lata Govada[a], Piyapong Asanithi[b], Emmanuel Saridakis[c], Izabela Jurewicz[b], Eric W. Brunner[b], Rajesh Ponnusamy[d], Jamie A. S. Cleaver[c], Alan B. Dalton[c], and Richard P. Sear[c] , [a]*Biomolecular Medicine, Department of Surgery and Cancer Oncology, Faculty of Medicine,Imperial College London, London SW7 2AZ, United Kingdom,* [b]*Department of Physics and Chemical and Process Engineering, Faculty of Engineering and Physical Sciences, University of Surrey, Guildford, Surrey GU2 7XH, United Kingdom,*[c]*Institute of Physical Chemistry, NCSR "DEMOKRITOS", Ag. Paraskevi 15310, Athens, Greece,* [d]*Institute of Biochemistry, University of Lubeck, Ratzeburger Allee 160, 23538 Lubeck, Germany*
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The use of porous materials as nucleants for protein crystallization have been well documented over the past decade. Harnessing this porosity alongside the surface chemistry has the potential to yield nucleants of greater efficacy. To this end, we report on the first use of carbon-nanotube-based films. The nanotubes induced crystal nucleation in the metastable zone of the phase diagram for a range of proteins including the targets 'Human Cardiac Myosin Binding Protein-C' (MyBPC) and 'Nonstructural Protein 9 of the Transmissible Gastroenteritis Virus'. Furthermore, crystals of 'MyBPC' diffracted to a resolution of 1.6 Å improving on the previous limit of 3.0 Å. Thus, nanotube-based films are very promising candidates for future crystallisation trials of intractable proteins.

Keywords: protein crystallization-1, nucleants-2, carbon nanotubes-3

FA5-MS38-P13

Attenuated Total Reflection-FT-IR Spectroscopic Imaging of Protein Crystallization. Naomi E. Chayen[a], Lata Govada[a], K. L. Andrew Chan[b], Roslyn M. Bill[c], Sergei G. Kazarian[b], [a]*Biomolecular Medicine, Department of Surgery and Cancer, Faculty of Medicine, Imperial College London, SW7 2AZ, United Kingdom,* [b]*Department of Chemical Engineering,*

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A method for identifying protein crystals based on Attenuated Total Reflection Fluorescence Transmission Infrared Spectroscopy (ATR-FT-IR) is presented [1]. This approach uses imaging, through a combination of chemical specificity and the visualizing capability and is complementary to detection of crystals using Ultraviolet (UV) light. ATR-FT-IR imaging was successfully applied to study the crystallization of several proteins simultaneously from six different solutions, using microbatch under oil. The technique is fast as it studies protein crystallization in situ and provides an opportunity to examine many different samples under a range of conditions. Studies applying this technique with other proteins are underway.

[1] Chan, K.L.A., Govada, L., Bill, R.M., Chayen, N.E. & Kazarian, S.G. *Analytical Chemistry* ,2009,81, 3769-3775

Keywords: protein crystallization-1, imaging-2, atr-ft-ir-3

FA5-MS38-P14

Experimental Minstrel HT UV: Automated Imaging of Protein Drops with UV Fluorescence. Max Petersen, Jian Xu, Michael Willis, *Rigaku Automation, Inc., USA*
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The Minstrel HT UV™ is a fully automated imager specifically designed for high-throughput ultraviolet and visible crystal imaging and monitoring of protein crystal growth. We have focused our research and development efforts on combing knowledge and skill of experts in optics, photochemistry, illumination, and automation to develop a custom solution that provides the highest sensitivity, the highest optical resolution, and the least photo damage to a protein sample. The result of this effort provides a substantial leap forward in imaging technology in both UV and visible color spectrum. The optimal balance of high resolution and depth of field for the crystallographic application allows for imaging of hanging drop, sitting drop, and microbatch experiments for all UV suitable plates. When combined with Rigaku's Gallery™ 700 incubators, the Minstrel HT UV provides around the clock unattended incubation at user defined temperature settings and inspection schedules. Image analysis and the associated data management are handled by a software environment that not only allows for scoring of imaging results, but also reporting and management of all relevant crystallization information. Validation studies for various representative protein crystallization experiments show how the Minstrel HT UV imaging system is able to cope with complex drops, providing researchers with a significant advantage in the detection of protein crystals.

Keywords: protein crystallization, automation, microscopes