presence of metallic copper, and to cuprite in the orange tesserae. These phases are responsible for both the colour and opacity of the samples. In this context, in addition to the redox conditions in kilns, the relationships between the precipitation of the above phases and differing amounts of copper and lead in the samples were also discussed.

Lastly, the similarity of the present results with those already reported in the literature indicates routine glass production processes, notwithstanding their different age and provenance.

Keywords: archaeometry. XAS, glass

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Using 2D detectors for x-ray imaging

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The unique properties of newer generation solid state 2D detectors - like the combination of high dynamic range, low background and high spatial resolution with no point spread broadening - offer the possibility for new imaging applications.

In this contribution we will show examples of non-destructive X-ray imaging applications with a PIXcel^{3D} detector that is based on the Medipix2 technology. Examples include imaging techniques based on transmission geometry, Bragg diffraction (X-ray topography) and non-coherent scattering effects. These imaging applications allow to combine traditional X-ray analysis with micro-structural investigations of the samples and the correlation with macroscopic material properties. Examples of organic samples and semiconductor materials will be shown.

Keywords: imaging

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Macromolecular crystallization: robotics, procedures and Innovations

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At the time of crystallization experiments the structure of a macromolecule is not known and hence an optimum strategy cannot be established. At the LMB, scientists can undertake initial experiments using a wide variety of conditions and robust automated procedures [1]. The procedures are straightforward, enabling LMB scientists to operate independently. We are continuously developing methods, like the Pi sampling [2] and devices to increase the chance of crystallization and crystal optimization. There are now different MRC crystallization plates that can be used on commercially available robots [3]. Also, we have created screens like MORPHEUS [4] to complete the formulation of commercial kits.

[1] D. Stock *et al. Prog. Biophys. Mol. Biol.* **2005**, *88*, 311-327. [2] F. Gorrec *et al. Acta D,* **2011**, *67*, 463-470. [3] F. Gorrec *et al. Poster presentation (www.swissci.com)*. [4] F. Gorrec, *J. Appl. Cryst.* **2009**, *42*, 1035-1042.

Keywords: macromolecular crystallization, screen, automation

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Utilization of desiccant for enhancing protein crystallization

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The vapor diffusion (hanging or sitting drop) technique is widely used in protein crystallization screens. In conventional vapor diffusion crystallization screens the concentration of protein usually increases from $0.5C_p$ (C_p: the initial protein concentration before mixing with the reservoir solution) to ~C_p. This limited concentration range reduces the probability of the solution being in the nucleation zone. If the protein concentration range is increased, we may expect to see a higher crystallization success rate.

Based on the above consideration, we proposed a new method to increase the concentration range in protein crystallization by using desiccant instead of the reservoir solution in the vapor diffusion technique[1]. Fig. 1 illustrates the difference in the arrangement of crystallization cells between the conventional and modified vapor diffusion methods.

Thirteen proteins were tested using the modified and conventional sitting drop methods. It was found that the improvement by using the modified method is strikingly significant. With consideration of the following features we recommend this modified method for practical protein crystallization screens. (1) Conditions under which drops remain clear in the conventional vapor diffusion method may yield crystals in the modified method. (2) The modified method can produce crystals from solutions with lower initial protein concentrations, which consumes less protein. It is always very difficult to produce protein samples at concentrations sufficient for crystallization trials. Using the modified method, we did not need to worry as much about the concentration of the protein during sample preparation. (3) The involved modification is very simple and efficient and can be applied without the need for large changes to the standard vapor diffusion protocol. The modification can also be integrated into automated systems. (4) Finally, the modified method reduces the cost of screening because no reservoir solution is necessary.

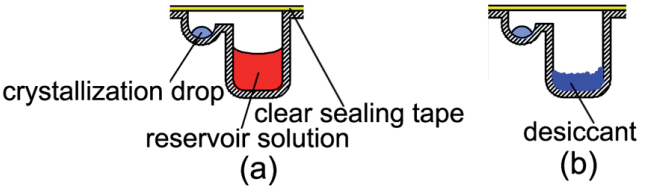

Figure 1. Schematic illustration of the difference in the arrangement of crystallization cells between the conventional and modified vapor diffusion methods. (a) The arrangement of crystallization cells in the conventional vapor diffusion method (sitting drop method). (b) The arrangement of crystallization cells in the modified vapor diffusion method[1].

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Keywords: protein, crystallization, methodology

MS92.P03

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Fields and crystals: what can we learn about quality?

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The use of electric and magnetic fields to improve the crystallization of protein crystals is not new. Different techniques have been discussed in the literature [1], [2], [3]. We will review these techniques and present new results obtained through the application of electrical fields using a novel device easily reproduced in the laboratory environment. The new device uses transparent conductive electrodes made by the deposition of ITO onto glass slides, and can easily be used in AFM scanning and topographic investigations. X-ray diffraction results will be compared to low magnetic fields attainable in the laboratory. In the end the question is if low electric or magnetic fields have an effect on crystal quality.

[1] H. Zoubida, S. Veesler, *Prog. in Biophys. and Mol. Biol.* **2009**, *101*, 38-44.[2] B.A. Frontana-Uribe, A. Moreno *Cryst. Growth and Des.* **2008**, *8*, 4194-4199.[3] A Moreno, F Yokaichiya, E DiMasi, V Stojanoff, *Ann. N.Y. Acad. Sci.*, **2009**, *1161*, 429-436.

Keywords: electric field, magnetic field, protein crystal quality

MS92.P04

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Random microseeding: a theoretical and practical exploration of the Microseed Matrix-Screening (MMS) method, with new recommendations for achieving crystallization success.

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Douglas Instruments has completed theoretical and practical studies of Microseed Matrix-Screening (MMS), a powerful approach to protein crystallization, introduced by Ireton and Stoddard in 2004 [1]. The method was automated by D'Arcy et al. [2], who first used seeding with random screening kits. Experience shows that MMS with random screens generates more hits or better-diffracting crystals in about 75% of cases where at least one crystal can be obtained.

Our studies included analysis of the stability of seed crystals suspended in unconventional stock solutions and the effectiveness of seed crystals from novel sources. This has given rise to new recommendations for maximizing the number of hits, reducing the prevalence of salt crystals, increasing the diversity of crystal forms, and harvesting seed crystals from microfluidic devices. We also investigated nucleation with microporous glass, zeolites, precipitates and mixtures of crushed crystals of proteins that were unrelated to the target protein. These were less effective than conventional MMS, but may still be useful - they can of course be used before the first hits have been found. Throughout the project, the statistical significance of experiments was increased by focusing on "pregnant" conditions - defined as conditions that reliably gave crystals when seeds were present, but which otherwise gave no crystallization.

References: [1] Ireton and Stoddard*, Acta Crystallographica* section D60 (**2004**)*, 601–605*; [2] D'Arcy et al. *Acta Cryst* D63 ***(2007)***.

Keywords: crystallization-1, microseeding-2, random-3

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Fluorescence anisotropy-based macromolecule crystallization screening

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Screening for protein crystallization is typically a highly digital process, with the screening results being interpreted as yes (a crystal) or no (no crystal). This approach leads to the routine setting up of hundreds or thousands of screening experiments to obtain the ever elusive crystal. However, there may be many screening outcomes that are close to crystallization conditions but which are discarded from subsequent consideration as they gave a clear or an amorphous precipitate result. A potentially better approach would be to first determine those conditions which are proximal to those necessary for crystallization, then concentrate on them for subsequent optimization rounds.

We are developing a fluorescence anisotropy-based screening method for just this purpose. The method measures the concentration-dependent changes in the rotational rate of the macromolecule in response to the test screening conditions. Difficulties in reproducibly pipetting sub-µL volumes led to inclusion of the intensity data as a quality check, and it rapidly became apparent that intensity also increased with likely, and found, lead conditions. The method is currently implemented using 1536 well plates, assay solutions consisting of 3 µof a solution composed of 0.6 µof protein solution and 2.4 µof precipitant solution. Eight solutions are used for each precipitant concentration; 1 buffer bland and 7 protein concentrations, typically ranging from 0.2 to 4.0 mg/mL. We are at present working on speeding up the data acquisition process (it currently takes ~1.5 hrs to acquire a data set) and reducing the assay solution volume, with our target volume being in the 10-20 nL range.

Keywords: screening, rapid, fluorescence

MS92.P06

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Structural and biochemical characterization of HP0315 as a VapD protein with an endoribonuclease activity from *Helicobacter pylori*

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Virulence associated protein D (VapD) found from various organisms, but not much information about VapD is known. Recently, the paper about novel ribonuclease family of Cas2 was reported and mentioned the relationship with VapD (1). Here, we show the first structure of a member of VapD and raise a theory about relationship among VapD, Cas2 family and toxin-antitoxin (TA) systems. The crystal structure of HP0315 from *Helicobacter pylori* was solved at 2.8 Å resolution with a modified ferredoxin-like fold. The structure of HP0315 is very similar to that of Cas2 family. Like Cas2 proteins, HP0315 has an endoribonuclease activity. HP0315 cleaved mRNA just before A and G nucleotides preferentially, which means that HP0315 has a purine specific endoribonuclease activity. Mutagenesis studies of HP0315 revealed several residues are important for RNase activity. HP0315 is arranged as an operon with HP0316 which recently was turned out to be antitoxin-related protein. However, HP0315 is not a component of TA system. HP0315 could be explained as an evolutionary