MS44-P3 **New modules for PiMS: data tracking of crystal handling protocols.**

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The Protein Information Management System (PiMS) is a well developed tool for following the molecular biology steps from construct design through to purified protein. xtalPiMS, built on PiMS, is a tool for managing crystallization experiments, and in particular the large numbers of images that can be produced by automated imaging systems. Like PiMS, xtalPiMS is a web-based application that runs on widely-available open source software; xtalPiMS is accessed using a web browser, typically requiring no additional software to be installed on the client. Current work on xtalPiMS aims to close the toolchain gap between the crystallization image of interest in xtalPiMS and the shipment of the crystal to the synchrotron with ISPyB, by providing a highly customizable and flexible method for recording crystal treatments. This work will provide a continuous record chain from protein sequence to X-ray diffraction images. xtalPiMS is available under the same terms as PiMS. To try xtalPiMS, visit http://pimstrak1.dl.ac.uk:8080/xtal/loginhome.jsp (user name "demo", password "demo").

Keywords: software; imaging; computer programs

MS44-P4 **X-ray Laue and Bragg diffraction on oxygen precipitates in annealed CZ-Si wafers.**

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We study structural properties of oxygen precipitates after various thermal treatment similar to microelectronic chip processing. The oversaturation of interstitial oxygen in Czochralski silicon results in formation of oxygen clusters which can deform the surrounding lattice as point defects. The presence of defects decreases the performance of fabricated integrated circuits, but on the contrary they can also be beneficial, since they can getter out impurities, such as heavy metal atoms. Such a lattice distortion influence stronly dynamical diffraction which is sensitive to size and volume of the deformed area in crystal [1].

In our experiment 2-3 mm thick Si wafers have been studied by x-ray diffraction in Laue geomery using Mo x-ray tube in order to involve large volume of defects in the wafer. All samples were preannealed at high temperature in order to eliminate temperature history during ingot cooling and further exposed to nucleaction and precipitation annealing. Time and temperature of thermal treatment differed in various samples.

The analysis of measured diffraction scans in Laue geometry was performed by means of Takagi equations and statistical dynamical theory of diffraction [1]. From the simulated Laue diffraction curves we find the size of the individual defect area and the fraction of strain area volume in the wafer. Diffraction reciprocal space maps in reflection Bragg geometry were also recorded, however only size of the defect can be estimated [2]. Results from bothe methods were compared.

Since the x-ray diffraction is not sensitive to the SiO_2 core but only to lattice strain, the results obtained from x-ray diffraction were supplemented by the loss of interstitial oxygen data according to infrared absorption spectroscopy. Combination of both techniques allowed us to estimate also the size of SiO_2 precipitate core where different defect sizes were obtained [3]. Systematic evolution of precipitate structural parameters was obtained according to various precipitation temperature and time. The concentration of defects increased in samples annealed longer and at lover temperatures and vice verse. The observed results were correlated also with transmission electron microscopy images and etch pit technique.

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