quality summing up in strain and geometrical behavior (Fig.1a). At the interface, dislocations in the annealed specimens (Fig. 1b) caused a broadening of the Si(333) reflection (Fig. 1c).

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Figure 1. Spatially resolved RCs for an as prepared specimen showing strain/tilt components (a). TEM picture showing dislocation density patterns (b). Reciprocal space map (RSM) on the Si(333) reflection from the annealed Si/Si interface (c), the dislocations caused a more diffuse Bragg-peak.

Keywords: reciprocal space mapping, stress analysis, bonded silicon, dislocations

## MS21-P2 Synthesis, structures and luminescence properties of two gallium(III) complexes containing 5.7dimethyl-8-hydroxyquinoline.

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Metal-quinolinates are known as key materials in the design of organic light emitting diode (OLEDs) devices since their discovery by Tang and Van Slyke back in 1987.<sup>1</sup> Quinolinol derivatives have been since envisaged as promising fluorophores. As a result, that has prompted growth in the science of these M(Ox)<sub>2</sub> entities with other icosagens down the boron group such as gallium (Ga) and indium (In).<sup>2.3</sup>Not only has there been extensive research on the structural discrepancies of these type of complexes leading to isomerization (*mer/fac*), but also, the net effect (in the solid state) imposed by the guest molecules trapped in the unit cell. Crystallography in particular, provided an excellent technique for the investigation of the net effect in these complexes w.r.t. to inter-molecular interactions therein and the solvento species "trapped" within the crystal lattice.<sup>4</sup>

In this work, two complexes of  $M(Ox)_3$  (M = Ga(III), OxH = 5,7 dimethyl-8-hydroxyquinoline) have been synthesized and characterized by <sup>1</sup>H NMR, <sup>13</sup>C NMR, single crystal X-ray Diffraction and SEM, and their photoluminescence properties evaluated. The fact that crystals were obtained with a different number of dichloromethane molecules in the crystal lattice, provides the rare opportunity to investigate solvent effects in photoluminescence.

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Figure 1. Crystallography as the decider in the optical behaviour of two gallium(III) complexes.



## MS21-P3 Phase transitions of silicon under dynamic and non-hydrostatic conditions

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Silicon represents one of the most important semiconductors in today's high-performance electronics. By the processing in the industry locally high pressures and temperatures emerge during the mechanical treatment and the wafer handling, leading to phase transitions under non-equilibrium conditions. This can result in a change of the electronic properties of the material, as well as the formation of cracks and the breaking of the wafers. We present time-resolved X-ray diffraction experiments under non-hydrostatic conditions that study in situ phase transformations of silicon. The experiments were conducted in a membrane-driven diamond anvil cell (mDAC) at the Extreme Conditions Beamline (ECB) P02.2 at PETRA III, DESY. We used powered Si standard and added gold flakes for pressure determination. The compression rates varied around 0.04 GPa/s and the maximal pressure went up to 20 GPa. Most experiments were conducted at room temperature. After one experiment, the sample was heated up to 500 °C using a graphite resistance heater. During compression and decompression, diffraction patterns were collected every 10 seconds. For analysis, three-dimensional contour plots were created to get an overview of the experiment to define the onset of phase transitions. In order to identify the phases and to determine the lattice parameters, we performed a LeBail analysis on single diffraction patterns. All experiments reveal two phase transitions during compression. Between 4 and 7 GPa, Si-I transforms to Si-II. The next phase transition from Si-II directly to Si-V occurs between 13 and 15 GPa, skipping the stability field of Si-XI. Si-V remains then stable to maximal pressure. Upon decompression, Si-V transforms to Si-III and Si-XII. The approximate proportion of Si-III to Si-XII is 20:1. The mixture remains stable to 2 GPa. At ambient pressure, this recovered sample was heated up to 500 °C to obtain Si-XIII. During heating, the two phases remain stable. Furthermore, there is no evidence that the proportion changes with respect to the diffraction patterns. However, a Raman-analysis of the recovered samples reveals a strong variation of this proportion over the entire sample. After maintaining at 500 °C for 5 minutes, two new reflections occur at low diffraction angles up to 11 °20 that can be indexed to Si-IV. However, two other strong reflections of this phase at higher 20-values are not observed. Being metastable, Si-IV could not identified by a Raman-analysis.

Keywords: Silicon, non-hydrostatic