



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

Keywords: Aluminium, Fluorescence, Quinolinol, Oleds

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 powdered 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 $11^\circ 2\theta$ that can be indexed to Si-IV. However, two other strong reflections of this phase at higher 2θ -values are not observed. Being metastable, Si-IV could not be identified by a Raman-analysis.

Keywords: Silicon, non-hydrostatic