

Report for the beamtime HS 3618:
Temperature Induced Phase Transitions of metastable Si and Ge modifications
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The data collection of the beamtime HS 3618 includes the measurements of the metastable high pressure modifications of Ge(*tP12*), Si(*cI16*) and BaSi₆ at high temperatures.

Analysis of the data at high temperatures of **Ge(*tP12*)** could identify the accompanying phases during the stepwise phase transition. Owing to the high resolution (and at the same time fast collected data) a more detailed investigation of the behavior directly at the starting of the phase transition was possible. Here for the first time intermediate phases during first order crystalline to crystalline phase transitions could be resolved. This unexpected result made visible by the high resolution of the ID31 serve as a basis for a further theoretical analysis by molecular dynamic simulations. The calculations are now finished and will be submitted together with the analysis of the powder diffraction data soon in the journal Nature.

The analysis of the collected data of **Si(*cI16*)** at high temperatures reveals that not only the crystallographic information has to taken into account but also a very difficult microstructure has to be analyzed. This problems leads to collaboration with the programmer Matteo Leoni (University of Trento) who develops one of the programs normally able to analyze such data. It turned out that no software is able to tackle the observed problems and more effort in the development of the program is now under way, together with molecular dynamics simulations, to handle and understand the observed changes of Si(*cI16*) at high temperatures.

The structure changes of the metastable high pressure compound **BaSi₆** could be resolved. Here three phase transitions could be detected and show for the first time that changes between silicon clathrate networks are possible. The publication is in preparation and will be submitted in the Journal of the American Chemical Society.