

**Experiment title:**

High-pressure EXAFS studies of Fe-and Ge-bearing amorphous and quasicrystalline materials

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HD-258

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Local contact(s):

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Report:

We conducted an extremely productive pilot study to develop the EXAFS techniques for the high pressure study of two archetypal 4th row elements: Ge and Fe. We looked at a number of model materials: Ge, GeO₂ glass, FeGeO₃, and (Fe_{0.4}Mg_{0.6})SiO₃. Crystalline elemental Ge has many pressure-induced phase transitions including metallization and electronic changes, and the well-known crystal structures from XRD provide a validation of the EXAFS approach. We studied this material to 60 GPa (Figure 1). The structure of glass GeO₂ has been studied by EXAFS to 29 GPa and XRD to 15 GPa. We extended the study of GeO₂ to 44 GPa over several increasing and decreasing pressure cycles (Figure 2). A number of structural and electronic transitions have been observed in FeGeO₃. Ge (Figure 3) and Fe (Figure 4) EXAFS of FeGeO₃ to 22 GPa provided element specific information through a transition that was observed at 20 GPa. (Fe_{0.4}Mg_{0.6})SiO₃ in post-perovskite structure plays a key role in the core-mantle boundary of Earth above 100 GPa. Its crystallinity disintegrates below 90 GPa but is poorly understood. This sample was especially challenging due to its thickness and the strong absorption by the diamonds anvils. We address these issues in our new proposal by using a stronger gasket and with the novel composite diamond anvils.

We are currently working on analysis of the results which is largely be conducted by Maria Baldini who is currently receiving training from Sakura Pascarelli in this area, and who will spend a month in ESRF in January 2009 to work on the results from this pilot study.

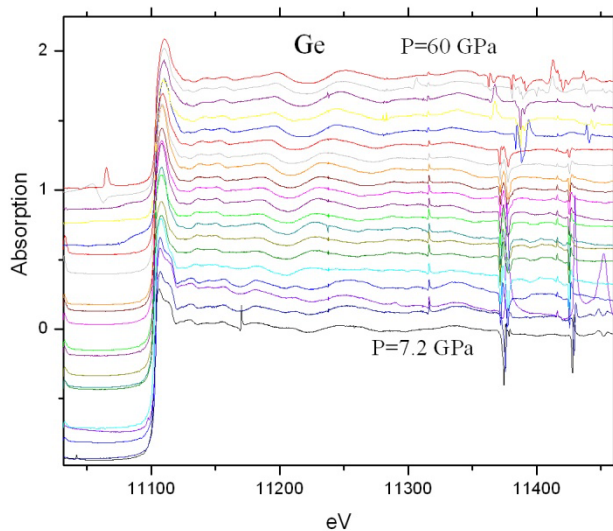


Figure 1. Ge EXAFS for crystalline Ge sample collected upon increasing pressure. The spectra correspond to from bottom to top: 7.2, 8.7, 9, 9.5, 10.5, 13, 13.9, 14, 15.8, 18.2, 20.9, 22.8, 25.3, 29.4, 35.2, 42.8, 47.6, 48.1, 52.4, and 60 GPa.

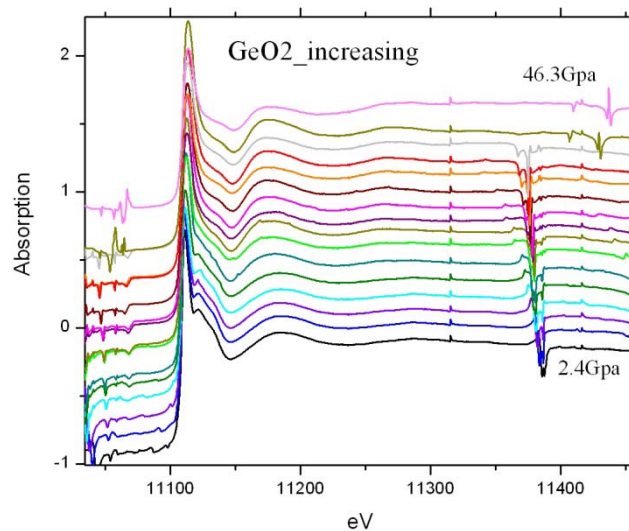


Figure 2. Ge EXAFS for amorphous GeO_2 sample collected upon increasing pressure. The spectra correspond to from bottom to top: 2.4, 4.9, 6.6, 6.8, 8.4, 10.5, 13.1, 16.7, 19.3, 22.2, 27.4, 30.2, 34.5, 38.8, 42.3, and 46.3 GPa.

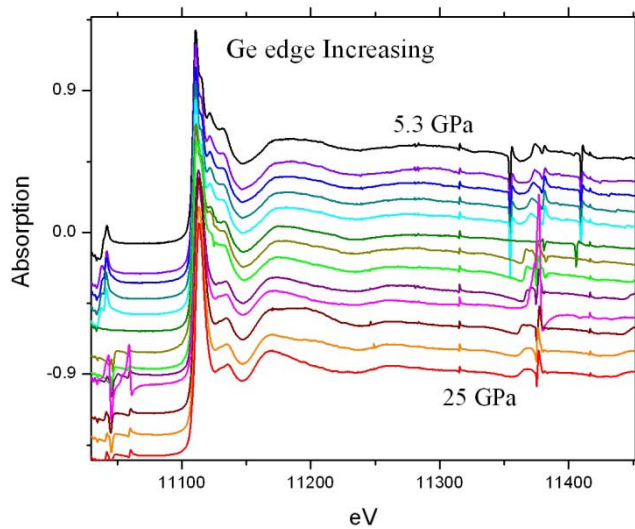


Figure 3. Ge EXAFS for FeGeO_3 sample collected upon increasing pressure. The spectra correspond to from top to bottom: 5.3, 6.9, 7.7, 8.4, 9.4, 9.6, 12.5, 14.2, 17.8, 19.8, 22.4, 23.3, and 25 GPa.

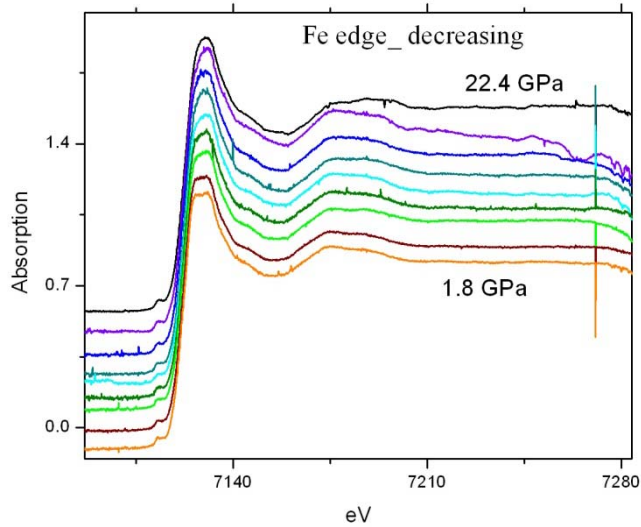


Figure 4. Fe EXAFS for FeGeO_3 sample collected upon decreasing pressure. The spectra correspond to from bottom to top: 1.8, 2.9, 6.4, 7.7, 9.3, 11.7, 14.2, 17.1, and 22.4 GPa.