	Experiment title: XAFS investigation of ion-implanted and adsorbed Xenon and Krypton in nanodiamonds and nanocarbons	**Experiment number**:
Beamline: ROBL-RCH	**Date of experiment**: from: 11.12.2017 to: 18.12.2017	**Date of report**: 01.03.2018
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Report:

Background.

Nanodiamonds and a poorly characterized carbonaceous matter, termed the Q-phase ("Q" stands for "quintessence") are the main carriers of isotopically-anomalous xenon observed in some primitive meteorites. One of the most remarkable features of Xe in meteoritic nanodiamonds is clear bimodality of their release pattern on heating: a so-called P3 fraction is released at 400-500 °C and the second one (the HL-component) at higher temperatures. Our recent studies of meteoritic carbonaceous matter highly enriched in the Q-component also indicate bimodality of the gaz release patterns.

Despite intense studies, no clear explanation of the bimodal Xe release patterns exist. Presumably, the P3 component reflects Xe trapped at surfaces of nanodiamond grains whereas the HL ions were implanted. Counterintuitively, implantation of monoenergetic Xe ions (700 eV) leads to the same bimodal Xe release pattern. Our recent in-situ TEM study of Xe implantation in nanodiamonds complemented by advanced molecular dynamics and quantum chemistry calculations (Shiryaev et al., in press) provide some hints, but still unambiguous determination of local environment of implanted Xe in nanodiamond and some other nanocarbons remains elusive.

Experiment

The proposed experiment aims at determination of Xe and Kr local environment in nanodiamonds and several astrophysically-relevant carbons using EXAFS. To be cosmochemically-relevant, we had to employ only low-energy ions and clearly absolute concentrations of the implant should be as low as reasonably possible in order to prevent amorphisation and other types of the samples' modification.

Furthermore, it is highly important to perform the experiment on loose nanoparticles (i.e. powder) rather than on nanocrystalline thin films.

Two sets of nanodiamonds with well defined grain sizes (5 and 40 nm), nanocrystalline diamond film, graphite, and several types of sp^2-nanocarbons were implanted using Kr/Xe plasma with energies up to 1500 eV and immediately packed. As a reference Xe adsorbed on zeolite and porous carbon was measured. At ROBL beamline XANES spectra at Kr and Xe K-edges were measured in fluorescence mode using a dedicated grazing incidence holder to address only very thin implanted layer (the implantation depth is 1-3 nanometers).

Results

Despite fairly low absolute concentrations of the implanted ions high photon flux available at the ROBL beamline allowed acquisition of distinct XANES spectra of the elements of interest, see Figure below.

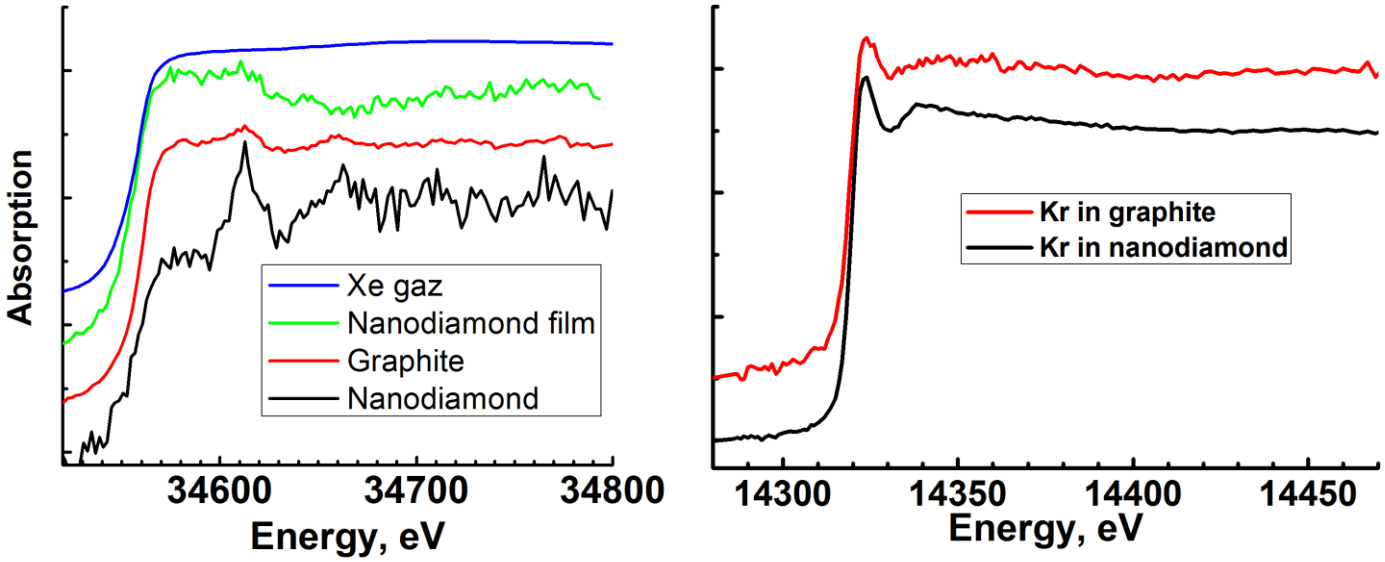

Figure 1. Typical XANES spectra of Xe and Kr in carbonaceous samples.

Clear differences in the XANES region are observed for various types of nanocarbons. Whereas in nanodiamond Xe and Kr may form complexes with vacancies, in graphite-like structures the most plausible trap for the implanted noble gases is the space between graphene sheets. However, since radii of Xe and Kr are larger than thet interlayer spacing, puckering of the sheets shoyld occur. Interestingly, Xe environment in nanocrystalline diamond film resembles that in graphite. The most plausible explanation of this behavious lies in complex structure of these nanocrystalline films, which consists of diamond grains envelopped into graphite-like shells.

At present we are performing detailed quantum chemistry calculations in order to derive a consistent model for behaviour of implanted noble gases in different types of nanocarbons.

We note here that the maximum ion fluence in our work was $5*10^{15}$ ions/cm^2 and it is well possible that a significant fraction of implanted ions was lost already during the implantation (e.g. ions trapped in pores between carbon grains). Despite the fact that the multi-element detector had to be positioned relatively far from the sample in order to avoid collision with the grazing-incidence holder, spectra acquisition was successful.The total area of every sample was approx. 1 cm^2; therefore, the experiment shows very high performance of the beamline.even