



	Experiment title: Dynamic behavior of overpressurized rare gas clusters	Experiment number: HS 60
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Names and affiliations of applicants (* indicates experimentalists):

* G. Faraci, * S. La Rosa, *A. R. Pennisi

Dipartimento di Fisica -- Universita' di Catania -- corso Italia 57,95129 CATANIA
ITALY

Report:

Si(111) single crystals and Be polycrystals were implanted at room temperature with Kr at 100 KeV with dose 10^{16} - 10^{17} atoms/cm²; the samples were also annealed in situ at 670 K for few hours and observed during the thermal treatment. During implantation the Kr beam at the specified energy penetrates about 100 nm into the matrix where its distribution follows a broad Gaussian profile.

X-ray absorption spectra were performed at the D32 beamline of ESRF (European Synchrotron Radiation Facility, Grenoble, France). This is a synchrotron radiation bending magnet source with a flux at the sample of 10^{11} photons/s and an energy resolution $\Delta E/E = 0.5 \cdot 10^{-4}$ for the Si(311) monochromator. The x-ray energy range used for our spectra was in the range 14100 - 14980 eV. As already mentioned, the samples contained a thin (100 nm) surface layer of implanted rare gas which therefore was observed by detecting the fluorescence photons produced by the x-ray beam. 5 Ge ultrapure photon detectors at 77 K were used to increase the counting rate within the discriminator window selecting the photopeak. A cryo-oven was employed to maintain the temperature of the sample at a fixed value in the range (83-670) \pm 1 K.

Some typical spectra are shown in Fig. 1. As evident in the figures, some marked near-edge structures are present in the raw spectra but no EXAFS oscillation is visible in the upper energy range, even at 83 K. This temperature is lower than the Kr melting point (117 K) at normal pressure and therefore Kr clusters are certainly solid. A simple observation confirm the presence of rare gas clusters. In fact, if the rare gas would be uniformly diffused into the matrix in atomic form without any kind of agglomeration, the shape of the x-ray absorption spectra would show the typical trend of Kr gas without any white line.

On the contrary, in our measurements all the spectra present a well shaped near-edge structure which can be attributed to continuum state transitions in Kr agglomerates. However, the absence of EXAFS oscillations can be explained by the following arguments: i) first of all, it depends on the very weak signal due to dilution of the rare gas clusters in the matrix; ii) second but most importantly it is related to the very fast decay of the back-scattering amplitude of the photoelectron wave from the Kr atoms around the absorber, mainly at intermediate temperatures where the atomic thermal motion smear out any interference effect. From the experimental spectra shown in Fig.1 it was possible to extract out of the noise valuable information contained in the near edge structures. In fact, we observe two peaks and a valley after the threshold, defined as the maximum of the first derivative; their energy position can be measured one respect to the other or with respect to the threshold. For a better resolution, we chose to measure the energy shift ΔE of the second peak from the threshold. We detected a value of ΔE increasing from 14.5 eV up to 18 eV in the Kr^+ implanted Be metal, and from 14 eV up to 15 eV for the semiconducting matrix. It is worth observing that at any temperature in both cases the threshold energy was very stable at 14336.2 ± 0.3 eV. This implies that the value of the measured shift is due to the temperature and is matrix dependent. This is also confirmed by the similar trend shown by the two samples. We mention that in order to improve the statistical accuracy several spectra were collected at a given temperature but no time dependence was observed in the spectra during accumulation; this exclude even at the maximum temperature (670 K) investigated any outgassing and/or any annealing effect. Another parameter deduced from the spectra is related to the relative amplitude between the maximum value h_{max} of the first peak and its valley h_{min} ; this was defined as: $\eta = 2(h_{max} - h_{min}) / (h_{max} + h_{min})$ so to obtain the height of the first oscillation with respect to the average. The experimental points decrease continuously from 0.35 to 0.13 for Kr/Be whereas the attenuation is somewhat reduced for Kr/Si from 0.29 to 0.17.

The significance of the previous parameters in relation to EXAFS results obtained for solid Kr thick films under high pressure at room temperature and for Kr solid crystal at 4.2 K, will be discussed elsewhere. Furthermore XANES calculations by using FEFF6 will be compared to both sets of data.

