Results of the EXAFS experiment 'Determination of Er sites in Er-implanted silica containing Si nanocrystals by means of EXAFS spectroscopy'.

Samples:

SiO_x (x<2) + annealing + Er implant ($5x10^{14}$ Er^+/cm^2)+annealing (900°C, 1h)
(RT, 800°C, 1250°C)
(19A, 21A, 23A)

SiO_2 with Si nc + Er implant + annealing (900°C, 1h)
$5.4x10^{19}$ Er/cm^3 (137B)
$2.1x10^{20}$ Er/cm^3 (119A)
$1.4x10^{21}$ Er/cm^3 (121A)

The EXAFS experiment was performed at the Italian beamline GILDA of the European Synchrotron Radiation Facility at the Er L_{III}-edge in fluorescence mode, cooling the samples at T=77K. The x-ray beam from a bending magnet was dynamically focused on the sample. The Er-Lα fluorescence signal from the samples was recorded by a 13-element high-purity Ge detector.

First shell analysis.

All the recorded EXAFS spectra exhibit one main oscillation (see Fig. 1), related to the Er-O coordination. Correspondingly, in the Fourier transform moduli of the spectra (see Fig. 2) the peak of the first coordination shell (Er-O) is clearly visible at about R~1.5-2Å.
The first shell analysis was performed exploiting the FEFF8-FEFFIT software package, fitting the first shell back-transformed signal (q-space), using the phase and amplitude calculated for the Er-O coordination of the $Er_2Si_2O_7$ model compound. In the Fig. 1, the comparison between the best-fitting curve and the experimental spectra is reported; the fitting results are collected in Table 1.

sample	Er-O		
	N_O	R (Å)	σ^2 ($\times10^{-4}$Å^2)
19A	2.2±0.4	2.05±0.01	60±27
21A	4.4±0.6	2.09±0.02	250±30
23A	3.5±0.5	2.10±0.02	189±30
137B	3.1±0.3	2.095±0.008	115±15
119A	5.8±0.2	2.161±0.003	240±7
121A	6.3±1.3	2.23±0.02	220±46
Er_2O_3			
site I	6	2.27	
site II	4	2.24	
	2	2.31	

It is found that:

- The Er-O coordination distance is always shorter than the corresponding average value for the crystalline Er_2O_3; the largest value is R=2.23Å, corresponding to the sample 121A.
- The coordination number is lower than that of the crystalline Er_2O_3, but for the 119A and 121A samples.
- There is a general correlation between the coordination number and the coordination distance, larger is the first, larger is the second (see Fig. 3).
- The effect of heating the substrate before the Er implantation is to increase the coordination number of O atoms around Er.
- The effect of increasing the Er implantation dose is to increase the coordination number of O atoms around Er.
- In Fig. 3 the results obtained (the red line is a guideline for the eye) are compared with those in literature for Er-implanted silica (Marcus et al, JNCS 91 and JNCS 96). Marcus et al. (JNCS96) found that in Er-implanted silica (flat-top profile, E~5MeV, top concentration = 1at%), the effect of annealing in vacuo (T=900C, 1h) is to increase the coordination number and the Er-O average distance from N=2.2, R=2.11 Å (marker c, Fig. 3) towards N=6.3, R=2.24 Å (marker d, Fig. 3). The same annealing did not turn out in significant structural modification if the Er concentration is lower (0.1at%, markers a and b).

Second shell analysis.

In most all the spectra a second shell is visible, located at about R=3 Å. The analysis of the signal from the first two shells was based on the GNXAS code, considering a model for the Er site in which each first-shell O atom is bonded with a Si atom in a typical SiO_2 tetrahedron. In the fitting, both the single scattering signals (Er-O and Er-Si) and the three-atoms scattering signal (from the Er-O-Si triangle) was considered. This model reproduces the experimental data of the samples 19A, 137B and 121A, as shown in Fig. 4.

Possible Er-Er coordination, if present, is below the detectable limit.

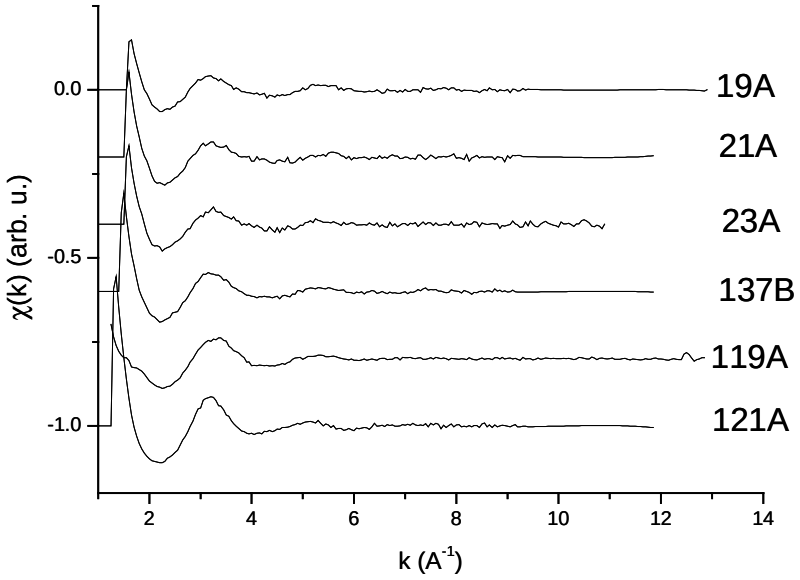
0.0
-0.5
-1.0
χ(k) (arb. u.)
2
4
6
8
10
12
14
k (A-1)
19A
21A
23A
137B
119A
121A

Fig. 1

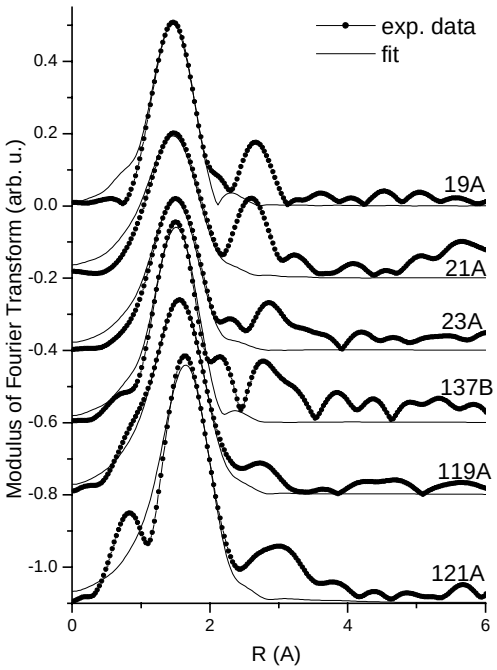
exp. data
fit
0.4
0.2
0.0
-0.2
-0.4
-0.6
-0.8
-1.0
Modulus of Fourier Transform (arb. u.)
0
2
4
6
R (A)
19A
21A
23A
137B
119A
121A

Fig. 2

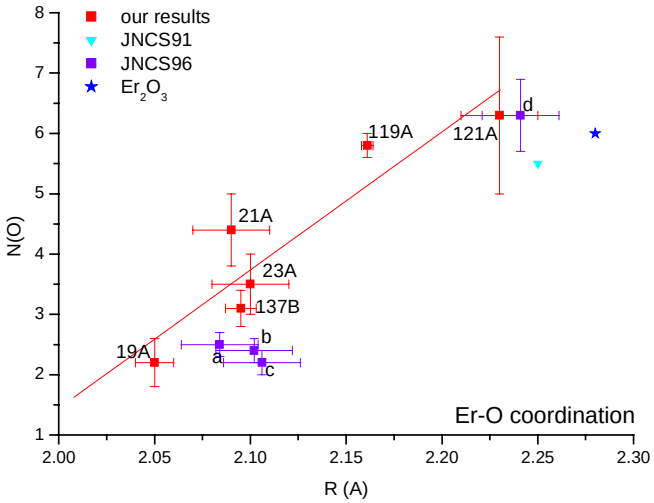
our results
JNCS91
JNCS96
Er2O3
N(O)
R (A)
Er-O coordination
19A
21A
23A
137B
119A
121A
a
b
c
d

Fig. 3