ESRF	**Structural origin of the dopant – induced stabilization of very high-κ ultra thin films**	**Experiment number**: 08-01-877
Beamline: BM -08	**Date of experiment**: from: 24/9/2010 to: 24/9/2010	**Date of report**: 30/8/2014
Shifts: 15	**Local contact(s)**: F. d'Acapito	*Received at ESRF:*

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Report:

Using x-ray absorption fine structure aided by ab initio structural simulations we demonstrate the atomic scale mechanism responsible for the stabilization of the otherwise unstable and very high-k tetragonal phase of ZrO_2 by the incorporation of Ge atoms. In tetragonal ZrO_2 the cation has a split first coordination shell formed by eight oxygen atoms. We provide a direct experimental proof that when Ge is incorporated in the oxide, four of the eight O atoms collapse towards Ge giving rise to a local structure strongly reminiscent of that found in quartz-like GeO_2, thus stabilizing the tetragonal phase.

Fig. 1 reports the local structure for Ge in ZrO_2 while Fig. reports the Ge EXAFS data.

These results have been published as:

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Atomic scale mechanism for the Ge-induced stabilization of the tetragonal, very high-κ, phase of ZrO_2

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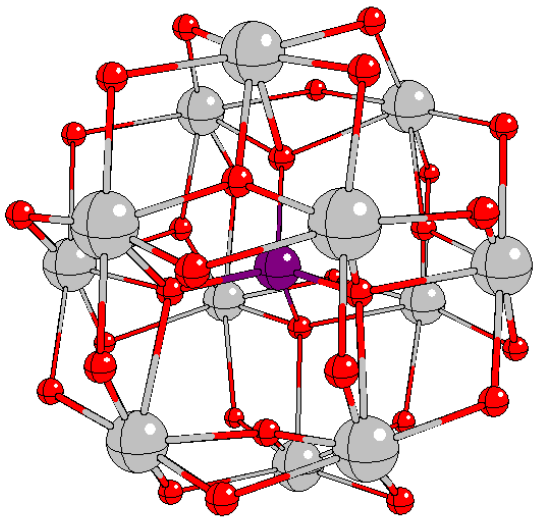

Fig. 1. Local structure of Ge in ZrO_2. The central purple atom is Ge, the small red atom O, and the large grey one Zr.

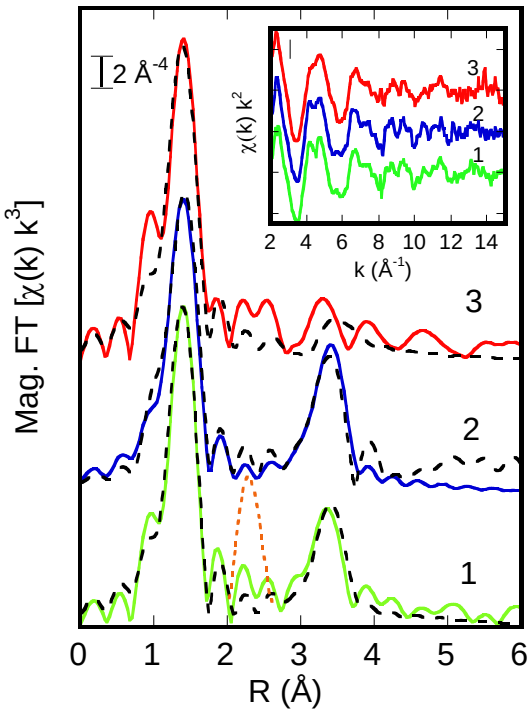

Fig. 2. Ge K-edge XAFS data for the three samples. The inset reports the background subtracted raw data. The main part of the figure reports as continuous lines the corresponding magnitude of the Fourier transforms while the long dashed lines are the fits.