ESRF	**Experiment title:** Atomic scale ordering in Pr - Y mixed oxide heterostructures	**Experiment number**: 08-01-884
Beamline: BM-08	**Date of experiment**: from: 23/2/2011 to1/3/2011 and from 20/4/2011 to 23/4/2011	**Date of report**: 26/2/2013
Shifts: 21	**Local contact(s)**: Francesco d'Acapito	*Received at ESRF:*

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Report:

Ternary single crystalline bixbyite $Pr_xY_{2-x}O_3$ films over the full stoichiometry range (x=0-2) have been epitaxially grown on Si (111) with tailored electronic and crystallographic structure. By performing extended X-ray absorption fine structure at both Y K and Pr L_{III} edges on the GILDA-BM08 beamline, in combination with complementary high resolution x-ray diffraction measurements, we have been able to perform a detailed study of the local atomic environment.

We have found that the local structure exhibits systematic variations as a function of the film composition, as illustrated by the spectra reported in Fig. 1. The cation coordination in the second and third coordination shells changes with composition and is equal to the average concentration, implying that the $Pr_xY_{2-x}O_3$ $Pr_xY_{2-x}O_3$ films are indeed fully mixed and have a local bixbyite structure with random atomic-scale ordering. A clear deviation from the virtual crystal approximation for the cation-oxygen bond lengths is detected, as illustrated in Fig. 2. This demonstrates that the observed Vegard's law for the lattice parameter variation as a function of composition is based microscopically on a more complex scheme related to local structural distortions which accommodate the different cation – oxygen bond lengths.

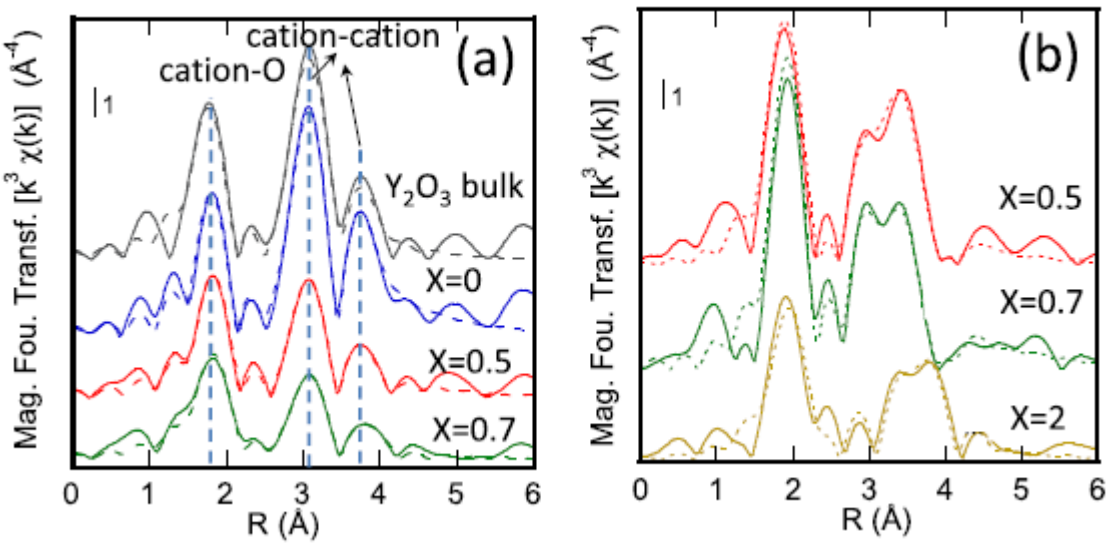

Fig. 1: Fourier transforms of Y K-edge and Pr L_{III} edge EXAFS data

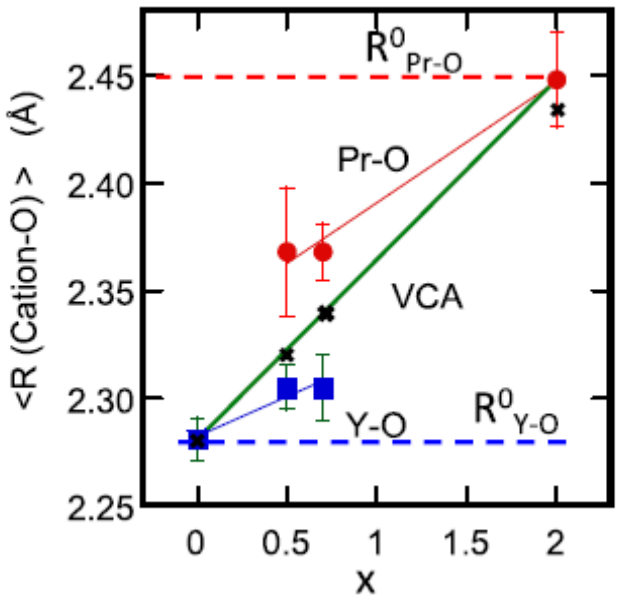

Fig. 2: Cation – oxygen bond lengths (symbols with error bars). The green line is the prediction of the virtual crystal approximation and the dashed lines are the composition – independent sums of ionic radii.

These results have been published in the paper: G. Niu et al., J. Appl. Phys. **113**, 043504 (2013).

JOURNAL OF APPLIED PHYSICS **113**, 043504 (2013)

X-ray diffraction and extended X-ray absorption fine structure study of epitaxial mixed ternary bixbyite $Pr_xY_{2-x}O_3$ ($x = 0–2$) films on Si (111)

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