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Cd-K Edge studies on II-VI semiconducting $Cd_{1-x}Ca_xO$

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Introduction

The CdO and CaO crystallize in cubic symmetry (F*m3m*) with similar lattice parameters 4.695 and 4.81 Å respectively. However, the variation of lattice parameter of the solid solution $Cd_{1-x}Ca_xO$ with x exhibits a negative quadratic deviation from the linear behavior (Vegard's law), characterized by a bowing parameter *b*=-0.031 Å. Though the solid solution has center of inversion, prominent Raman modes are observed for 0≤x≤1. These observations indicate that local symmetry deviates from the average symmetry as revealed by X-ray Diffraction studies. In view to study the local structure and its evolution with x, Cd-K edge extended X-ray absorption fine structure (EXAFS) measurements on $Cd_{1-x}Ca_xO$ at ambient conditions were carried out at NW-10A beam line, Photon Factory (PF-AR), Tsukuba.

Results and discussions

Standard procedures were employed to align the Cd-K absorption edge to reference material and pre- and post-edge subtraction of the absorption curve using Athena programme [1] The Fourier transformed χ(k) weighed by k^3 is shown in fig. 1.

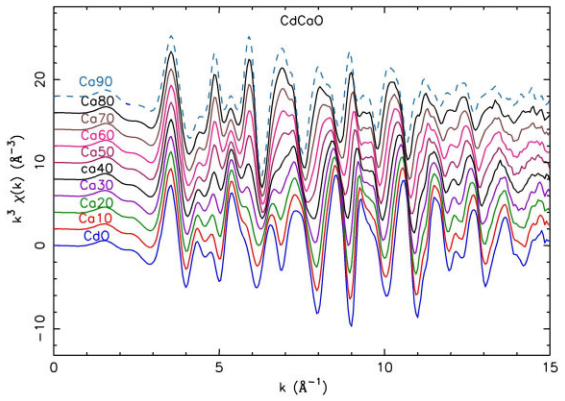

Fig. 1. k^2 weighted EXAFS χ(k) curve vs k for $Cd_{1-x}Ca_xO$. Curves are vertically shifted for clarity.

Continuous evolution of signal as a function of x is seen in the range for 4≤k≤13. This indicates modifications in the local structure with Ca substation, which has larger ionic radius compared to that Cd. Fourier transformed χ(k) signal is shown in Fig. 2. The first peak ~ 2.33 Å correspond to first nearest neighbour (*nn*) Cd-O distance, while the peak about 3.3 Å correspond to2 nn Cd-Cd/Ca distance.

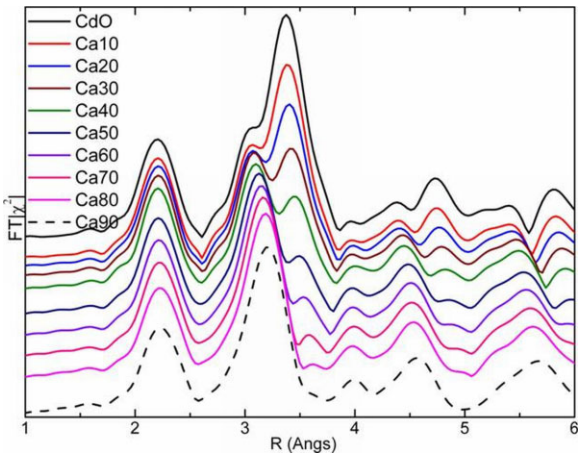

Fig. 2. Fourier transformed χ(k) curve for $Cd_{1-x}Ca_xO$ system

The shell by shell fitting in the real space was carried out using ARTEMIS programme [1] with a weighting factor 3 and including phase correction. It is seen that end-member CdO itself exhibits finite local deviations from the average cubic structure, with a reduction in the *1nn*) distance (d_{Cd-O}) by ΔR1=- 0.015(2) Å and with disorder, σ_o^2 = 0.0073(1) $Å^2$. With substitution of Cd, the 1-nn also non-linearly increases while associated disorder marginally. The non-linear dependence of 1-nn distance was fitted to a second order equation, yielding a bowing parameter b=0.02 Å. The 2-nn (Cd-Cd/Ca) also increases non-linearly but with much smaller.

This study clearly indicates local structure about Cd differs from average structure. The first nearest neighbour distance variation mimics the lattice parameter variation with Ca substitution.

Reference

[1] M. Newville, J. Synchrotron Rad. **8**, 322 (2001).

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