



Experiment title: Atomic ordering and local strain in the ZnSSeO quaternary alloy

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08-01-720**

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Report:

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F. Boscherini, M. Malvestuto, G. Ciatto, F. D'Acapito, G. Bisognin, D. De Salvador, M. Berti, M. Felici, A. Polimeni, and Y. Nabetani, "X-ray absorption and diffraction study of II-VI dilute oxide semiconductor alloy", *Journal of Physics: Condensed Matter* **19**, 446201(2007).

Abstract:

Dilute oxide semiconductor alloys obtained by adding oxygen to a II–VI binary compound are of potential applicative interest for blue-light emitters in which the oxygen content could be used to tune the band gap. Moreover, their properties can be usefully compared to the more thoroughly studied dilute nitrides in order to gain insight into the common mechanisms which give rise to their highly non-linear physical properties. Recently, it has been possible to deposit ZnSeO and ZnSeOS epilayers on GaAs(001), which exhibit a red-shift of the band gap and giant optical bowing.

In order to provide a structural basis for an understanding of their physical properties, we have performed a study of a set of ZnSeO and ZnSeOS epilayers on GaAs by high resolution x-ray diffraction and x-ray absorption fine structure.

We have found that the strain goes from compressive to tensile with increasing O and S concentration and that, while all epilayers are never found to be pseudomorphic, the ternary ones exhibit a low relaxed fraction if compared to the ZnSe/GaAs sample. O K-edge x-ray absorption near edge spectra and corresponding simulations within the full multiple-scattering regime show that

O is substitutionally incorporated in the host lattice. Zn and Se K-edge extended x-ray absorption fine structure detect the formation of Zn–O and Zn–S bonds; the analysis of these spectra within multiple-scattering theory has allowed us to measure the local structural parameters. The value of Zn–Se bond length is found to be in agreement with estimates based on models of local distortions in strained and relaxed epilayers; an increase of the mean square relative displacement is detected at high O and S concentration and is related to both intrinsic and extrinsic factors.