XAFS Study of $ZnSe_xTe_{1-x}$ Sinusoidally-modulated Superlattices

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Introduction

The possibility of creating semiconductor superstructures with controlled parameters opens up opportunities for observing new physical phenomena and technological applications. By MBE deposition of $ZnSe_{0.5}Te_{0.5}$ on GaAs (001) it has been established through x-ray diffraction and TEM that a superlattice is formed of $ZnSe_xTe_{1-x}$, with *x* varying sinusoidally with depth, with a period of about 30 Å, depending on growth conditions.[1] It is unclear whether the modulation in the electronic density detected by XRD is due to redistribution of the Se and Te atoms with depth, or whether it is just a strain wave with no exchange of the atom positions. Using the ability of XAFS to selectively probe the environment of a specific atom type and the selective in-plane ot out-plane sensitivity depending on polarization, we are attempting to resolve this issue and provide insight into the underlying mechanism causing the formation of the superlattice.

Methods and Materials

The samples are 5mm by 15mm glass slides covered with a thick GaAs wafer miscut at an angle, over which $ZnSe_{0.5}Te_{0.5}$ is MBE deposited using a commercial Riber 32 R&D system. A series of samples at various miscut angles were prepared and were studied with XRD. The 0, 3 and 4 degree miscut samples were used for Se K-edge polarization dependent XAFS measurements at the MRCAT 10-ID ID line. Liquid nitrogen temperatures were maintained to minimize thermal disorder with a specially designed sample chamber described elsewhere [2]. Measurements were made at different incidence and azimuthal angles to eliminate diffraction peaks.

For calibration standards used in the XAFS analysis, ZnSe MBE-deposited standards using the same Riber 32 system were used and XAFS parameters used in fitting of the samples were extracted. The 0 deg sample, which is a random $ZnSe_{0.5}Te_{0.5}$ alloy and was verified with XRD, was also used to calibrate the model.

MRCAT beamline is equipped with a double-crystal cryogenic Si (111) monochromator and tunable undulator which allows XAFS measurements over the energy range from 5 KeV to 30 KeV. A harmonic rejection mirror was also used to eliminate the third and higher x-ray harmonics from the monochromator; the contamination of the beam by these higher energies greatly complicates the data interpretation. XAFS data were obtained in fluorescence and TEY mode on all samples. The gas used in the TEY detection was 100% He, and in fluorescence, 100% N_2.

Model

A linear, single-scattering model combining second-shell XAFS from the Se environment in each of the layers within a superlattice period was used. Data was simulated with FEFF 6.0.1 [3] for a sinusoidal modulation of the composition *C(z)* and the distance between layers, *d(z)*, both in-phase, with the period of the superlattice. A schematic of the model is shown in Fig. 1. The results of the simulations are shown in Fig. 2.

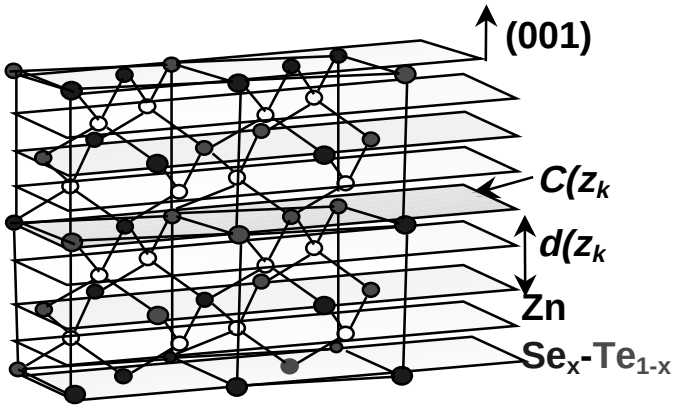

Fig. 1. Schematic of alloy structure used in modeling the composition and strain modulation.

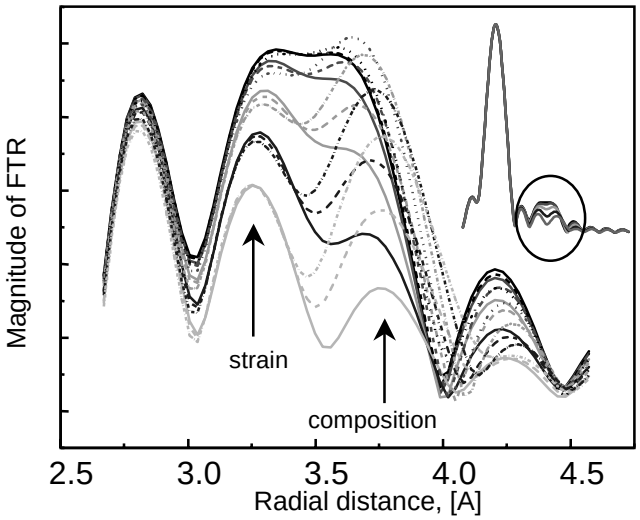

Fig. 2. Results of FEFF simulation of XAFS Fourier transform magnitude. Lines of same color are iso-'strain wave amplitude', lines of same type are iso-'composition wave amplitude'.

As can be seen in Fig.2, clear and systematic differences can be observed for ±20% sinusoidal variations in the distance and composition from the random $ZnSe_{0.5}Te_{0.5}$ alloy.

Results and Discussion

The reduced XAFS spectrum and it's Fourier transform are given in Fig. 3 below. Using the reference standards, XAFS parameters for the Se environment were determined which were later used to fit the above spectrum using FEFFIT [4]. Results from fitting indicate that both a strain and a composition wave are present, with amplitudes of about 0.05A in distance difference from the $ZnSe_{0.5}Te_{0.5}$ alloy and about 3% in compositional difference (i.e. $Se_{0.47}$-$Te_{0.53}$ to $Se_{0.53}$-$Te_{0.47}$). Unfortunately, relatively large scan-to-scan variations in data do not allow precise determination of

error bars, as well as some of the correlations between the variables in the fit.

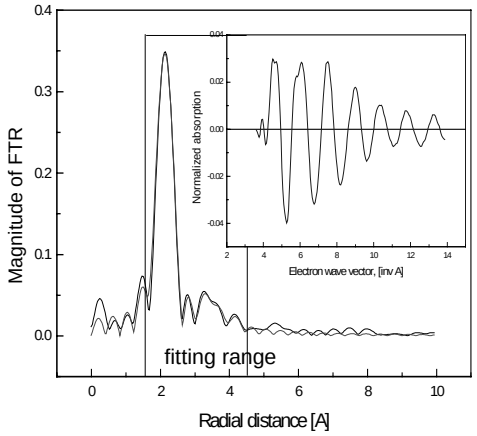

Fig. 3. XAFS data from ZnSeTe superlattice. Inset: XAFS oscillations, $\chi(k)$. Full frame: Fourier transform magnitude.

Conclusions

XAFS measurements were done in TEY/fluorescence mode on a $ZnSe_xTe_{1-x}$ MBE deposited superlattice and standards at the MRCAT beamline of the APS. A sinusoidal composition and strain model was developed, tested and applied to the measurements and preliminary results on the amplitude of the waves obtained. Indications are that both strain and composition waves with depth are present, with small amplitudes. More repeatable data is needed, however, for the conclusive determination of these parameters.

Acknowledgments

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