

EXAFS Study of As-Doped HgCdTe

B.D. Chapman,¹ E.A. Behne,¹ G.T. Seidler,^{1,2*} P. Boieriu,³ S. Sivananthan³

¹Department of Physics, University of Washington, Seattle, WA, U.S.A.

²PNC-CAT Sector 20, Advanced Photon Source, Argonne, IL, U.S.A.

³Department of Physics, University of Illinois, Chicago, IL, U.S.A.

Introduction

The semiconducting alloy HgCdTe (MCT) is an interesting system because its tunable, narrow band gap makes it an ideal material for infrared detector and diode laser applications. While MCT-based infrared technology continues to evolve toward increasingly complex device structures, there is a pressing need for improved doping profiles and doping levels on the p and n sides of junctions. Arsenic has become a prime choice as a p-type dopant, and its incorporation into HgCdTe layers during molecular beam epitaxy (MBE) growth has been demonstrated.¹ However, the As-doped HgCdTe layers show highly compensated n-type properties. The source of this behavior does not appear to be associated with As dopants but rather unidentified structural defects acting as donors.² Extended x-ray absorption fine structure (EXAFS) measurements are uniquely suited to probe the local atomic structure in these systems. We present EXAFS measurements of the As and Hg local environments in MBE-grown HgCdTe layers with *in situ* As incorporation.

Methods and Materials

All measurements were made at the Pacific Northwest Consortium Collaborative Access Team (PNC-CAT) insertion device beamline (sector 20-ID). Energy selection was achieved using a liquid-nitrogen-cooled double-crystal Si(111) monochromator, with the second crystal detuned $\sim 30\%$ for harmonic rejection. Both the As K-edge (11868 eV) and Hg L_{III}-edge (12284 eV) EXAFS were measured for three HgCdTe:As samples, with As-dopant content: 10^{20} , 10^{19} , and 10^{16} cm⁻³. The sample preparation method is described elsewhere.³ The Hg_{1-x}Cd_x alloy composition of these samples is $x = 0.17$, and the thickness of the films is ~ 2.5 μm . The samples were under ambient conditions. The incident signal was monitored with a helium-filled ion chamber, and the fluorescence yield from the sample was measured with an argon-filled ion chamber. The effective As K α fluorescent signal was $\sim 10^7$ p/s, and typical spectra were obtained in ~ 1 hour. Background subtraction was performed using AUTOBK.⁴ Fourier transforms to R-space were done using k^2 weighting and Hanning windows, over the range $k = 3.5$ \AA^{-1} to $k = 9.5$ \AA^{-1} and to $k = 10.5$ \AA^{-1} , for the As and Hg edges, respectively.

Results

Figure 1 shows the measured fluorescence yield for the 10^{20} cm⁻³ As-doped HgCdTe sample for both the As K- and Hg L_{III}-edges. The close proximity of the two absorption edges limits the spectral range of the As K-edge EXAFS signal, but we find that this limitation is currently only problematic in the low As concentration data. The As EXAFS signal after background subtraction is shown in Fig. 2 for the most concentrated sample. Figure 3 shows the Fourier transforms of both the As and Hg EXAFS for this sample.

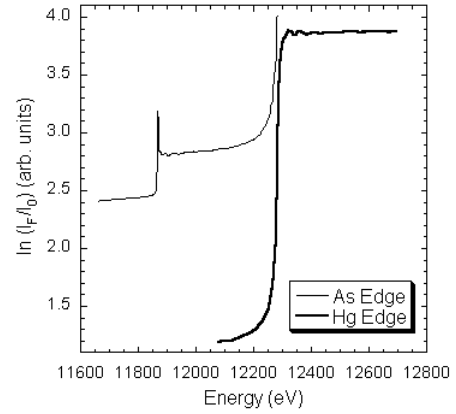


FIG. 1. Raw data: As K-edge and Hg L_{III}-edge absorption measured by fluorescence of HgCdTe:As with As-dopant concentration 10^{20} cm⁻³.

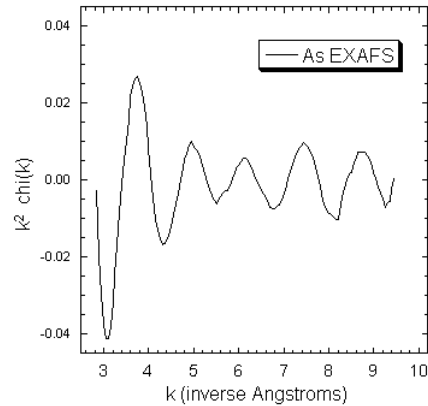


FIG. 2. Arsenic EXAFS of HgCdTe:As with As-dopant concentration 10^{20} cm⁻³.

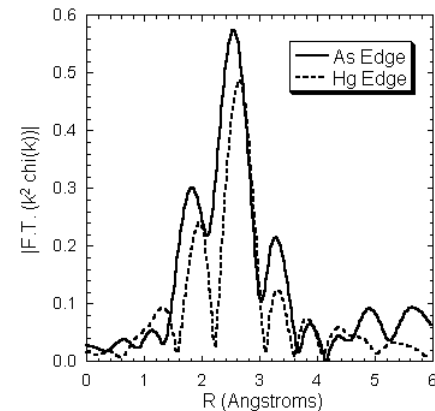


FIG. 3. Fourier transform of the As K- and Hg L_{III}-edge EXAFS of HgCdTe:As with As-dopant concentration 10^{20} cm⁻³.

Discussion

We are presently investigating self-absorption effects in the EXAFS signals and modeling the data with the theoretical standards of FEFF7⁵ for a more quantitative determination of the local atomic structure. Comparisons to the *ab initio*, quasi-thermodynamical models of Grein et al.¹ will be made, and detailed results will be published soon.

For future data collection, we intend to use a fluorescence detector with energy discrimination in order to increase the spectral range of the As K-edge data past the interfering Hg L-edges. This will also increase the EXAFS quality in the low As content measurements.

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- * Author to whom correspondence should be addressed: seidler@dirac.phys.washington.edu