

	Experiment title: Study of the site-specific activation of As as an acceptor in HgCdTe	Experiment number: 30.02.704
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Experiment

The experiment was very difficult to conduct. First of all, the Ge substrate fluorescence completely blackout the As fluorescence so that we had to rip off the As:HgCdTe layer from all our samples before measurements. The very small amount of powder obtained made it very difficult to find any As signal. The As signal-to-noise ratio obtained was small despite all precautions we took: fluorescence detector as close as possible, lead or aluminum nose to avoid diffusion signal, use of Ge and/or Hf 3 μ and 6 μ filters. Therefore, we were not able to record any reasonably good spectra for any of the fully qualified samples where As concentration is below 1.10¹⁸cm⁻³. As a consequence, we had to grow in urgency some fall-back samples, where As was incorporated at a much higher level (>10¹⁹cm⁻³) on a Ge-free ZCT substrate using a brand new As plasma cell. The signal-to-noise ratio was then very good and we were able to fully determine chemical environment of As.

Results

Figure 1 compares $k\chi(k)$ EXAFS oscillations for sample A and B while Figure 2 compares $|\chi(R)|$. As can be seen on Figures 1&2, there is a major effect of thermal annealing on EXAFS oscillations. Figure 2 shows this is associated to the dominant contribution (first double peak between $R \in [1.4-2.8\text{\AA}]$) becoming single and a second peak around $R=3.4\text{\AA}$ appearing: annealing leads to complete change in As chemical environment as well as a better ordering around Arsenic. As first peak between $R \in [1.4-2.8\text{\AA}]$ is double, Arsenic (in not-annealed sample) has two different environments: EXAFS oscillations are made of the 2 same contributions but with different amplitude: the low-k contribution (k value below vertical bar) is more intense for sample B that sample A and vice-versa for the high-k contribution.

EXAFS analysis was conducted on the Fourier back-transformed oscillations $\text{Re}[\chi(q)]$

taking into account only the dominant R contribution and fit adjustments values are given in Table 1. As a consequence of the reduced available k-range, we had to limit the number of adjustment parameters for the 2 contributions of not-annealed sample. We choose to have a single energy offset E and a single Debye-Waller σ^2 parameter for both contributions. Also, it was not possible to have a sufficiently correct fit for the peak at $R=3.4\text{\AA}$ for annealed A&B. Figure 3 shows comparison between experiment and fit, agreement between experiment and fit being excellent.

For each adjustment, a small and rather constant energy shift $E(\text{eV})\approx 4\text{eV}$ was found, consistent with neutral As. EXAFS analysis clearly identifies the 2 contributions: a first one comes from Te being at 2.65\AA giving rise to the low-k contribution while the second one from As being at 2.46\AA and giving rise to the high-k contribution. As expected, amplitude of the Te contribution is larger for sample B than for sample A.

The first contribution indicates that As has incorporated inside HgCdTe in a mercury site, which is precisely one the expected results of this experiment. In the case of a single contribution, As should have 4 Te as first neighbors. Therefore, mercury substitution only concerns $1/5^{\text{th}}$ of Arsenic in sample A and $1/3^{\text{th}}$ in sample B. As (Hg,Cd)-Te distance in HgCdTe is 2.78\AA , this substitution occurs with a 1% contraction of bond length. To demonstrate more clearly the substitutional nature of As on mercury site, applicants have tried to find a second shell to As made only of 12 $(\text{Hg}_{0.7},\text{Cd}_{0.3})$ neighbors around 4.55\AA , but the much more intense second contribution prevented us to succeed.

This second contribution is made of As as first neighbors, indicating that most incorporated As are linked to another As. This may be the answering the long pending question of the nature of electrically inactive As.

Once annealed, only Arsenic neighbors are visible, in large number with an average distance of 2.5\AA indicating the formation of sub-cluster of Arsenic inside HgCdTe. Also, Debye-Waller σ^2 parameter increases from 3.10^{-3}\AA^2 to more than 7.10^{-3}\AA^2 , indicating the formation of an amorphous As sub-cluster: we were not able to show that the As activation process corresponds to As moving from mercury to tellurium site.

These results will be presented during the international conference on II-VI compounds.

Conclusion and prospects

Conducted experiments were able to show that part of As probably incorporates in mercury site and that electrically inactive As may be characterized by As having As as first neighbor. As successful recording of good quality spectra required As concentration above 10^{19}cm^{-3} , annealed sample where only made of As sub-cluster so that we were not able to show that the As activation process corresponds to As moving from mercury to tellurium site. Therefore, we believe that EXAFS is really the tool of choice to study the site-specific activation of As but we have to conduct this experiment using lower doped sample. To make it successful, we are now able to grow much thicker and larger sample on ZCT substrate allowing grazing incidence measurement and with the help of more flux using 200mA mode, we believe EXAFS recording of good quality spectra will be possible.

<i>R</i> range of back-transform	Nature	Number	Distance (Å)	σ^2 (10^{-3}Å^2)	<i>E</i> (eV)
[1.5:3.0Å]	Before annealing				
Sample A					
First contribution	Tellurium	0.85 ± 0.2	2.65 ± 0.05	3.0 ± 2	4.7 ± 1.3
Second contribution	Arsenic	2.0 ± 0.5	2.46 ± 0.02	same	same
Sample B					
First contribution	Tellurium	1.3 ± 0.1	2.63 ± 0.01	3.2 ± 0.5	3.2 ± 0.3
Second contribution	Arsenic	1.6 ± 0.1	2.46 ± 0.01	Same	Same
[1.4:2.8Å]	After annealing, $k > 4.4$				
Sample A	Arsenic	4.6 ± 1.5	2.49 ± 0.06	7.4 ± 3.4	4.9 ± 3.8
Sample B	Arsenic	7.2 ± 2.6	2.52 ± 0.07	10.3 ± 3.9	5.7 ± 4.2

Table 1: Adjustments values for data fit of As:HgCdTe samples A and B. S_0^2 was fixed to 0.8.

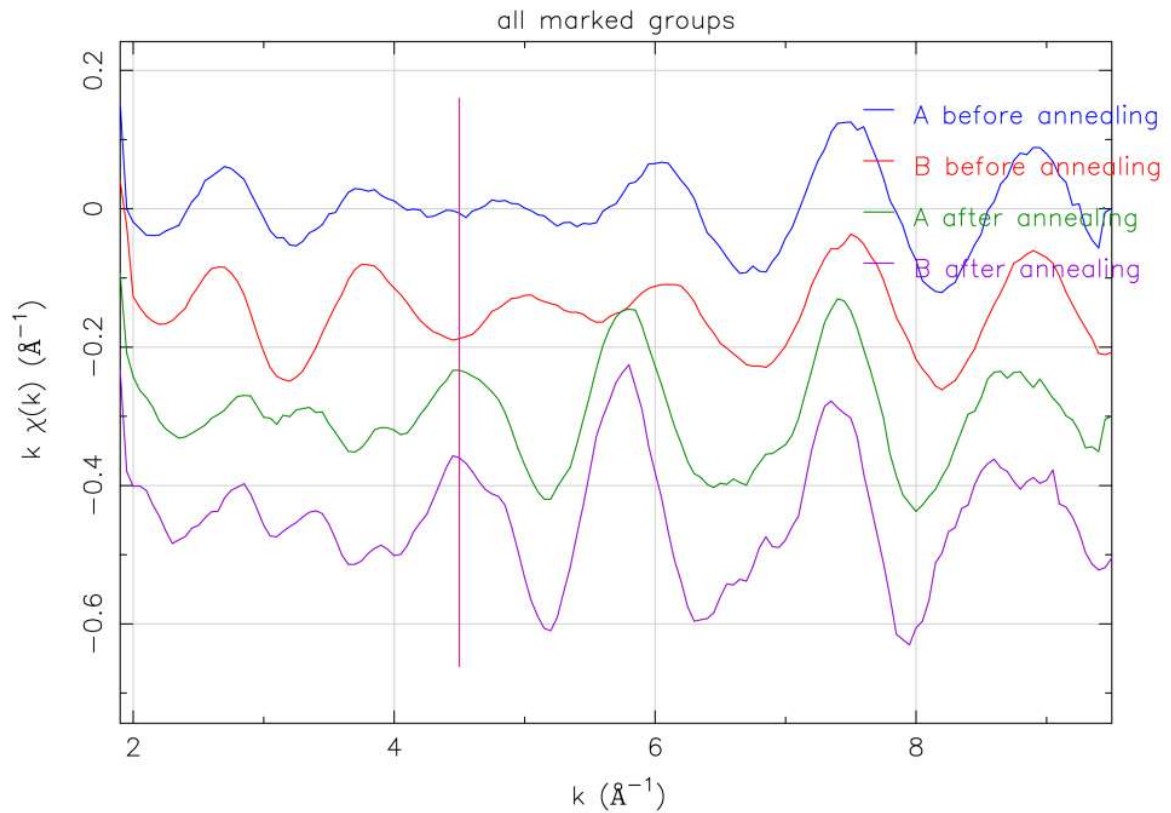


Figure 1: Comparison between EXAFS oscillations $k\chi(k)$ for samples A and B before and after annealing. Curves have been displaced by 0.15 vertically for clarity. The vertical bar at $k=4.5$ shows the limit between low- k and high- k contributions

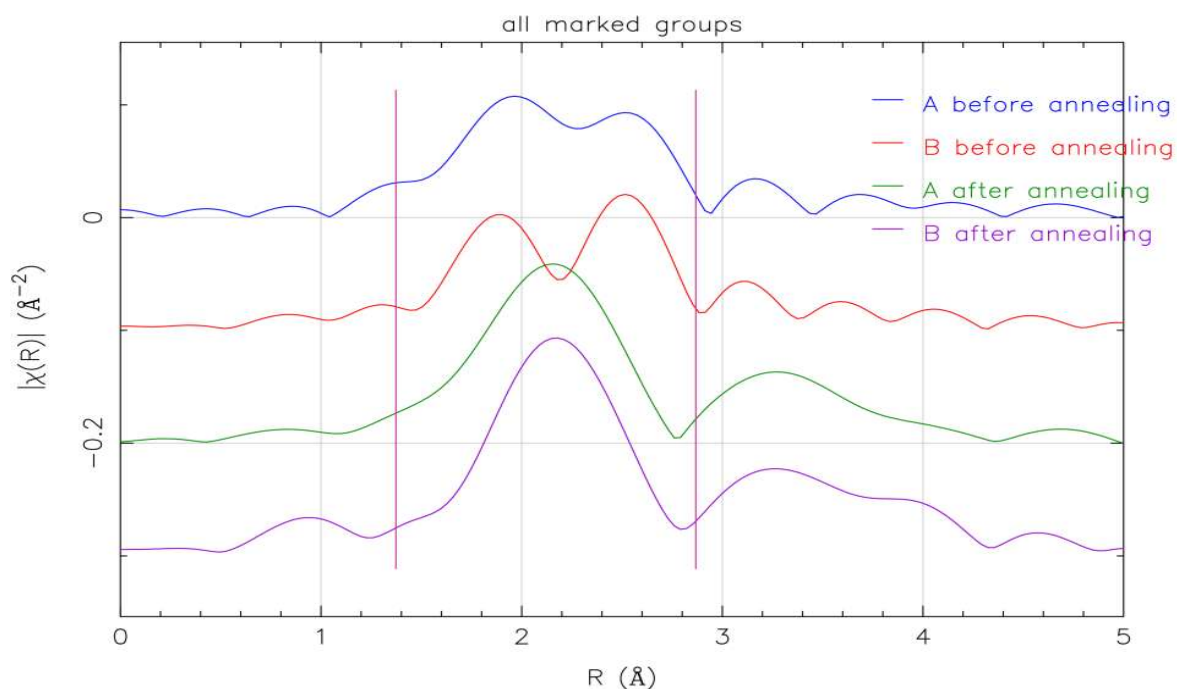


Figure 2: Comparison between EXAFS oscillations $|\chi(R)|$ for samples A and B before and after annealing. Curves have been displaced vertically by 0.1 for clarity. The vertical bars shows the R range taken into account for data fitting. $|\chi(R)|$ is not phase-corrected

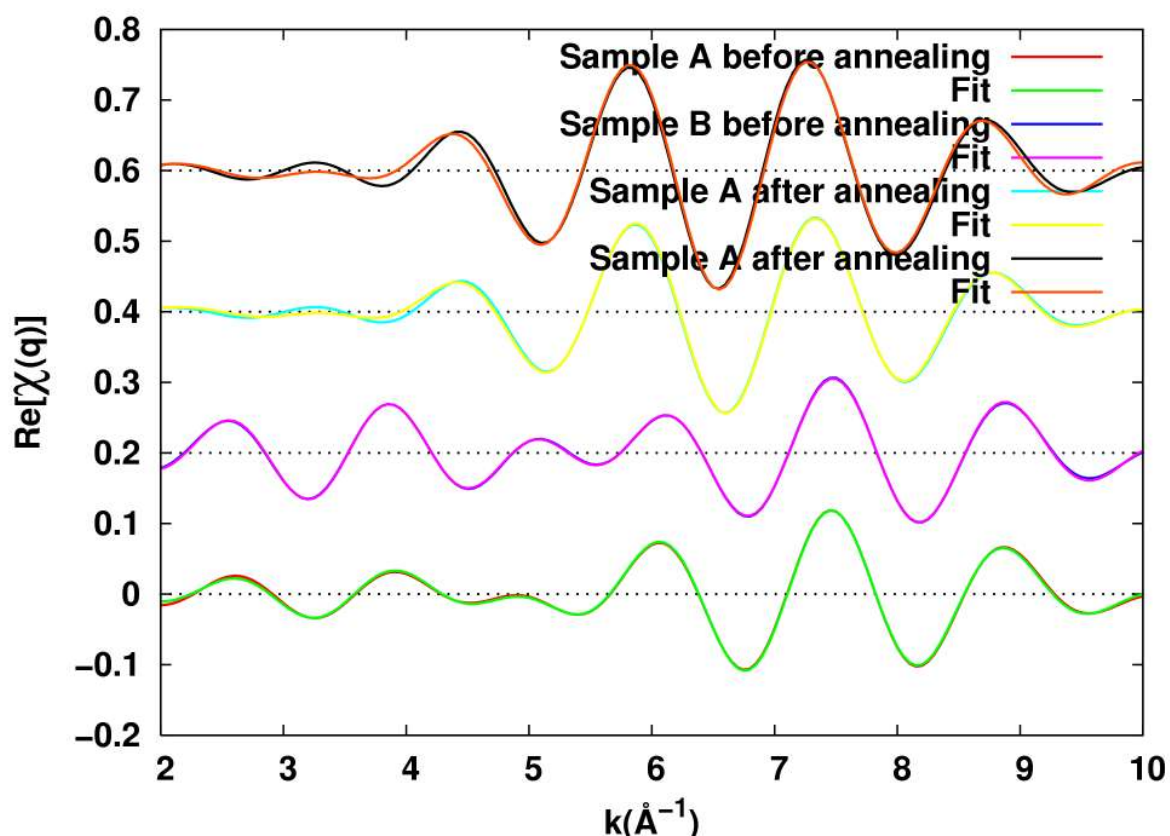


Figure 3: Comparison between EXAFS oscillations $|\chi(q)|$ and fit for samples A and B before and after annealing. Curves have been displaced vertically by 0.2 for clarity.