ESRF	**Experiment title:** *Investigation of the Pt impurity site configuration and Pt/Indium Selenide interfaces formation by means of fluorescence detected EXAFS*	**Experiment number**: HS-2568
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Report:

The aim of the experiment was studying the process of the Pt/InSe barrier formation at the atomic level by measuring the XANES and EXAFS spectra of Pt atoms deposited on InSe clean surfaces by fluorescence detected XAS, at different Pt coverage levels.

Large single crystals of non-doped InSe were grown by the Bridgman method. High quality samples with mirror-like surfaces can be prepared by cleaving the layered monocrystals. Samples for the experiment were prepared in an ultra-high-vacuum evaporation chamber connected to an XPS-UPS system. Samples were cleaved in vacuum and the amount of Pt on each sample was controlled by the relative intensity of Pt 4f core level peaks with respect to In 3d peaks. A series of samples with Pt coverages ranging from 0.2 to 5 mono-layers (ML) was prepared. Each sample was cut into 4 pieces and 3 of them were annealed in high vacuum at temperatures of 500, 600 and 700 K for 4 hours. All sample preparation was done during the two weeks just before the experiment.

The fluorescence-detected XAS experiments were performed at the Pt LIII absorption edge (11564 eV), by using a silicon diode placed perpendicular to the X-ray beam, in order to minimize elastically scattered radiation.

The Pt fluorescence signal was detected even at the lowest coverage rates (around 0.2 ML), for which the Pt atom areal concentration on the InSe surface is of the order of $2x10^{14}$ cm^{-2}, just above the detection limit of ID26. The PT LIII edge step was only 2% of the total signal and the EXAFS oscillations could not be extracted from the background noise. For Pt coverage rates larger than 0.5 ML XANES and EXAFS spectra can be extracted with a signal to noise ratio improving with the coverage rate. For the highest studied coverage rate (about 3 to 4 ML) the Pt edge step was about 80% of the background signal and high quality XANES and EXAFS spectra could be measured, with an energy range up to 700 eV above the Pt LIII absorption edge.

Figure 1 shows the XAS spectra of 4 samples (curves A,B,D,E), with the same Pt coverage rate (about 3 ML), each of them annealed at a different temperature. As expected, the spectrum of the non annealed sample is identical to the one of metallic platinum.

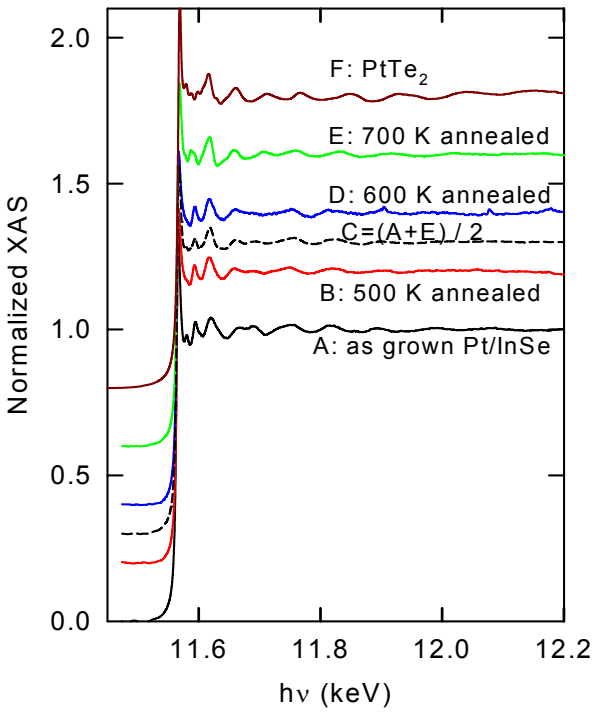

Figure 1: Normalizaed XAS spectra of 3 ML of Platinum on InSe for different annealing temperatures

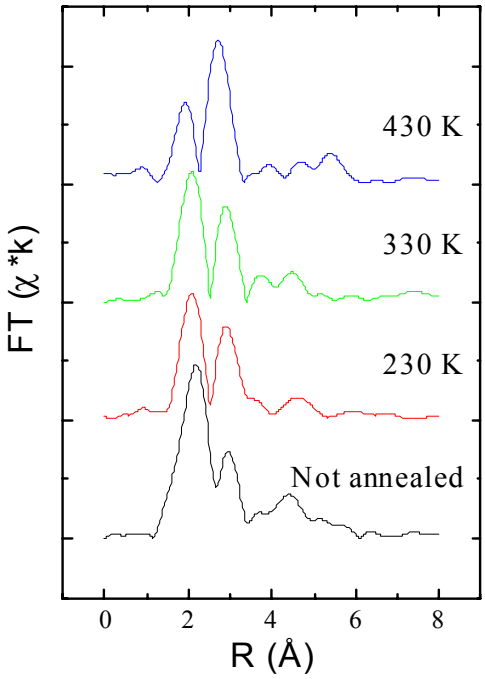

Figure 2: FT of spectra A, B, D and E in Fig.1.

The XAS spectra of annealed samples are different even for relatively low annealing temperatures, suggesting that Pt atoms diffuse into InSe even at relatively low annealing temperatures. In fact, from the evolution of the UPS/XPS spectra, Pt diffusion seems to occur even at ambient temperature. At the highest annealing temperature the spectrum is completely different both in the XANES and EXAFS regions.
The central spectrum in Fig. 1 (C) is just the average of spectra A and E. This average spectrum turns out to be nearly identical to spectrum B, which suggest that after annealing at 500 K around 50% of the Pt atoms are still at the surface as metallic Pt, while the rest have diffused into InSe.
Figure 2 shows the result of the Fourier transform of the EXAFS spectra of curves A, B, D and E in Fig. 1. This result indicates a decrease of the bond distance from the Pt atom to its first neighbors. This is what one should expect when the Pt atom coordination changes from the 12-fold compact one in metallic platinum to a lower 6-fold octahedral coordination like the one in interlayer sites in the InSe matrix. In order to check this hypothesis, XAS spectra of model compounds were taken. These compounds are the layered Pt chalcogenides PtS_2 and $PtTe_2$ in which Pt is an octahedral coordination similar to the one we propose for Pt in the InSe matrix. Curve F in Fig. 1 corresponds to the XAS spectrum of Pt in $PtTe_2$. In spite of the different anion, the similarity of spectra E and F is striking and supports the model of Pt diffusion to octahedral interlayer sites in InSe.
The XAS spectra of annealed samples with lower Pt coverage follow a similar trend and are similar to spectrum E in Fig. 1. For non-annealed samples the XAS spectra structures are broader than those in Fig. 1, but they turn out to be closer to those of annealed samples, indicating that, at low coverage rate, most Pt atoms diffuse into InSe. No clear trace of metallic Pt is detected in these samples.
In conclusion, the basic hypothesis of the proposal seems to be confirmed by the experiment.
Many spectra recorded during the experiment are still being interpreted. On the basis of these results, we are writing a paper on the formation of the Pt/InSe interface. A further set of results on Au/InSe interface was also obtained at the end of the experiment. Even if these results are less concluding (due to the closeness of the Se K-edge) we think that they will yield a coherent model when combined with XPS/UPS data.