Electronic Supplementary Material (ESI) for RSC Advances

Nanogravimetric study of lead underpotential deposition on selenium thin films as a semiconductor alloy formation procedure

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Supplementary Information

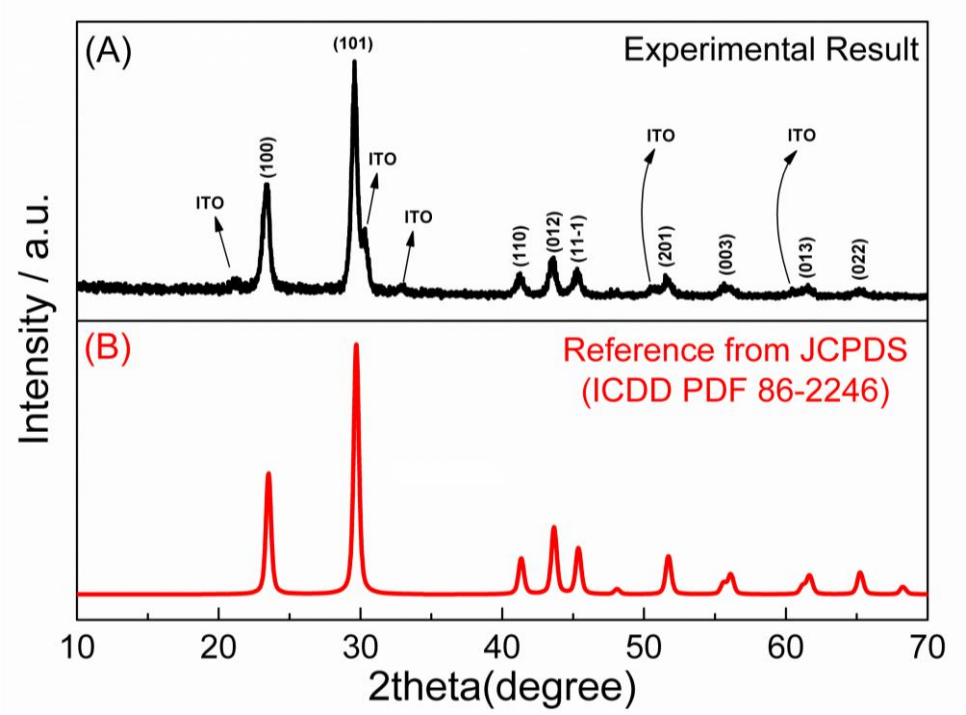

Fig. S1. X-ray diffraction patterns of a Se film deposited onto a conductive glass substrate (A) and the reference peaks obtained from JCPDS for Se (ICDD PDF 86-2246).

In Fig. S1 is presented the X-ray diffraction patterns obtained for a selenium film deposited onto a conductive glass substrate. In the same Figure the diffraction patterns of a reference (Se, ICDD PDF 86-224) obtained from JCPDS is also presented for convenience. The X-ray analysis showed that the obtained sample is a multi-phase with polycrystalline Se as the main phase. Additionally to the selenium pattern, other peaks also contribute for the multi-phase profile composition as indicated by the arrows in Figure S1 (A), which were easily associated with the ITO substrate (ICDD PDF 88-773).

In order to further confirm the structural features above discussed the Checkcell software [1] was used to analyze the XRD response of the Se film in order to evaluate the crystallographic orientation, the space group and the network parameter of the film components. The results presented in Table S1 shows that there is a good agreement between experimental and reference data confirming that Se deposited onto the ITO substrate as a polycrystalline film with hexagonal orientation (P3121 space group).

Table S1. Structural parameters for the Se thin film evaluated from XRD data

Material	Network Parameter			System	Space Group
	a	b	c		
Se	4.3748	4.3748	4.9575	Hexagonal	P3121
Se (pdf#86-2246)	4.3680	4.3680	4.9580	Hexagonal	P3121

The hexagonal closest-packed (hcp) unit cell considered for Se thin film is shown in Figure S2. The calculations carried out to obtain the density of the unit cell can be found elsewhere [2].

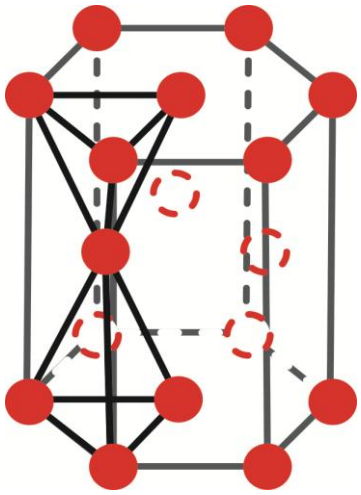

Fig. S2. The hexagonal closest-packing unit cell used to calculate the surface concentration of Se atoms per cm^2.

In order to calculate the density of Se atoms per cm^3, the concentration of atoms per cm^2 and the number of mols of Se per cm^2, the relationship using Avogadro´s law were used. To correlate the density of atoms per cm^3 and the concentration of atoms per cm^2 was used a relationship described in Ref. [3].

References

1 J. Laugier, B. Bochu, Checkcell – A Software Performing Automatic Cell/Space Group Determination, Collaborative Computational Project Number 14 (CCP14), Laboratoire des Matériaux et du Génie Physique de l'Ecole Supérieure de Physique de Grenoble (INPG), France, 2000.

2 B. S. Kelly, A. G. Splittgerber. J. Chem. Educ. 2005, 5, 756.

3 A. de Siervo. Determinação estrutural de ligas metálicas de superfície via difração de fotoelétrons.2002. 131 f. PhD Thesis - Instituto de Física “Gleb Wataghin” Universidade de Campinas, Campinas, 2002.