Surface X-Ray Diffraction study of a bi-layer junction based on Cu and Cd sulphides for photovoltaic applications

Tommaso Baroni*, Francesco Di Benedetto, Andrea Giaccherini, Enrico Berretti, Francesca Russo, Annalisa Guerri, Massimo Innocenti, Francesco Carlà, Roberto Felici
‘What’s really warming the world’
(CdS)$_{60}$/Ag(111) structure vs N° Cu$_2$S cycle

(012)$_{\text{CdS}}$ $l$-scan

$I (\text{r.l.u.})$

$\bar{l} = 2.330 \pm 0.003$ r.l.u.

(012)$_{\text{CdS}}$ $k$-scan

$k (\text{r.l.u.})$

$\bar{k} = 0.667 \pm 0.003$ r.l.u.
Greenockite
$P6_3mc$

\[
\begin{align*}
  a &= b = 4.137 \, \text{Å}; \\
  c &= 6.714 \, \text{Å} \\
  \alpha &= \beta = 90^\circ; \\
  \gamma &= 120^\circ \\
  V &= 99.52 \, \text{Å}^3
\end{align*}
\]

(CdS)$_{60}$/Ag(111)

\[
\begin{align*}
  a &= b = 4.332 \, \text{Å}; \\
  c &= 6.075 \, \text{Å} \\
  \alpha &= \beta = 90^\circ; \\
  \gamma &= 120^\circ \\
  V &= 98.73 \pm 0.37 \, \text{Å}^3
\end{align*}
\]
(0 0.73 0.2-6)_{Cu_2S} \textit{l-scan} and Cu_2S cell parameters

\begin{align*}
\text{(Cu}_2\text{S)}_{60}/\text{(CdS)}_{60}/\text{Ag(111)}_{\text{MA}3071} & \\
\quad & \\
\quad & a = b = 27.41 \pm 0.04 \text{ Å}; \quad c = 6.76 \pm 0.03 \text{ Å} \\
\quad & \alpha = \beta = 90^\circ; \quad \gamma = 120^\circ \\
\quad & c_{\text{chalco}} = 13.494 \text{ Å}
\end{align*}
Conclusions

- MA3071 is the first in-situ SXRD experiment which features an E-ALD bi-layer junction of Cu$_2$S/CdS/Ag(111).

- The SXRD in-situ analysis highlights the profound epitaxial relationship existing between the films and the bulk, consequent to the homogenisation of the metrics of the CdS and the Cu$_2$S structures to values commensurate to the surface periodicity of the substrate.

- The (CdS)$_{60}$/Ag(111) develops an elementary cell with crystallographic axes parallel to those of the surface cell of the Ag(111); the comparison with the structure of greenockite suggests a compensation mechanism related to the strain imposed by the film growth on the crystallographic Ag(111) surface.

- The positions in the reciprocal space of the Cu$_2$S reflections is compatible with an pseudo-hexagonal pattern rotated by 30 ° with respect to the surface cell cell of the substrate; the data suggest a hexagonal chalcopyrite-like structure with a planarization of the S layers, as a result of the strong epitaxial relationship existing with the CdS below and as already noticed in relation to a Cu$_2$S/Ag(111) E-ALD deposit by Giaccherini et al. (1).

- This study confirms E-ALD as an energy efficient method for the growth of semiconducting heterostructures with tailored properties using low cost/environmental-impact materials.