CIWC-2 2020

2nd Coatings and Interfaces Web Conference

15–31 May 2020

Chaired by Dr. Alessandro Lavacchi, Prof. Dr. Andriy Voronov

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

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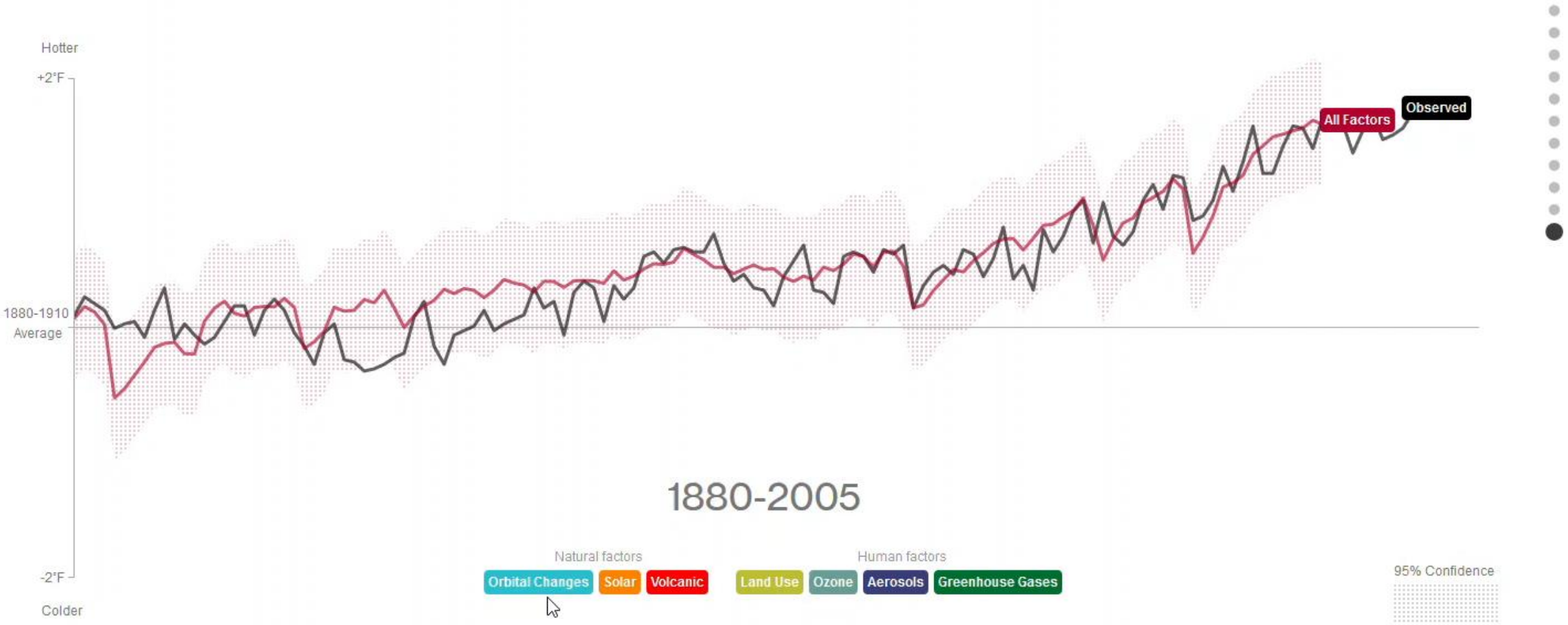
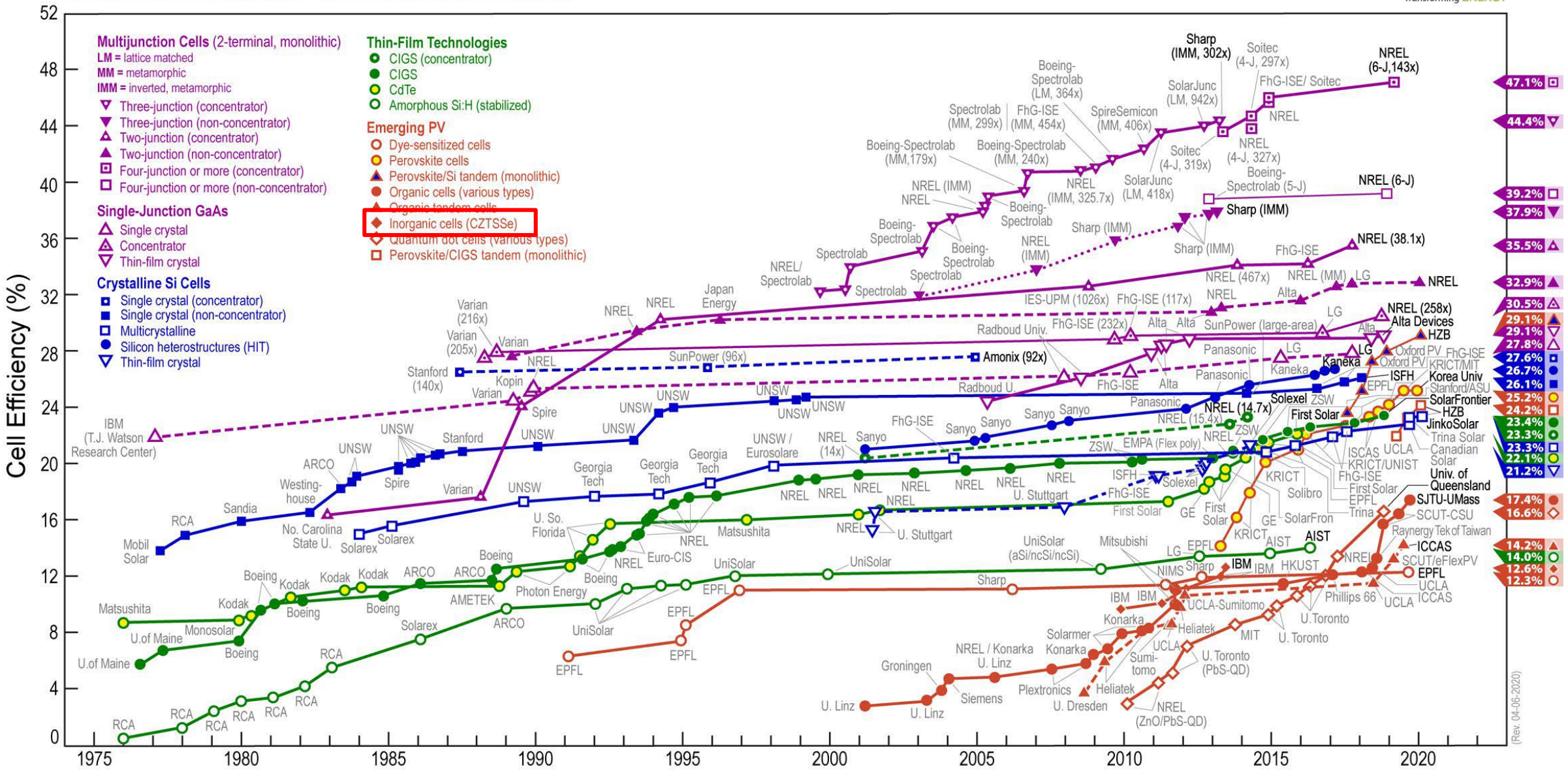
'What's really warming the world'

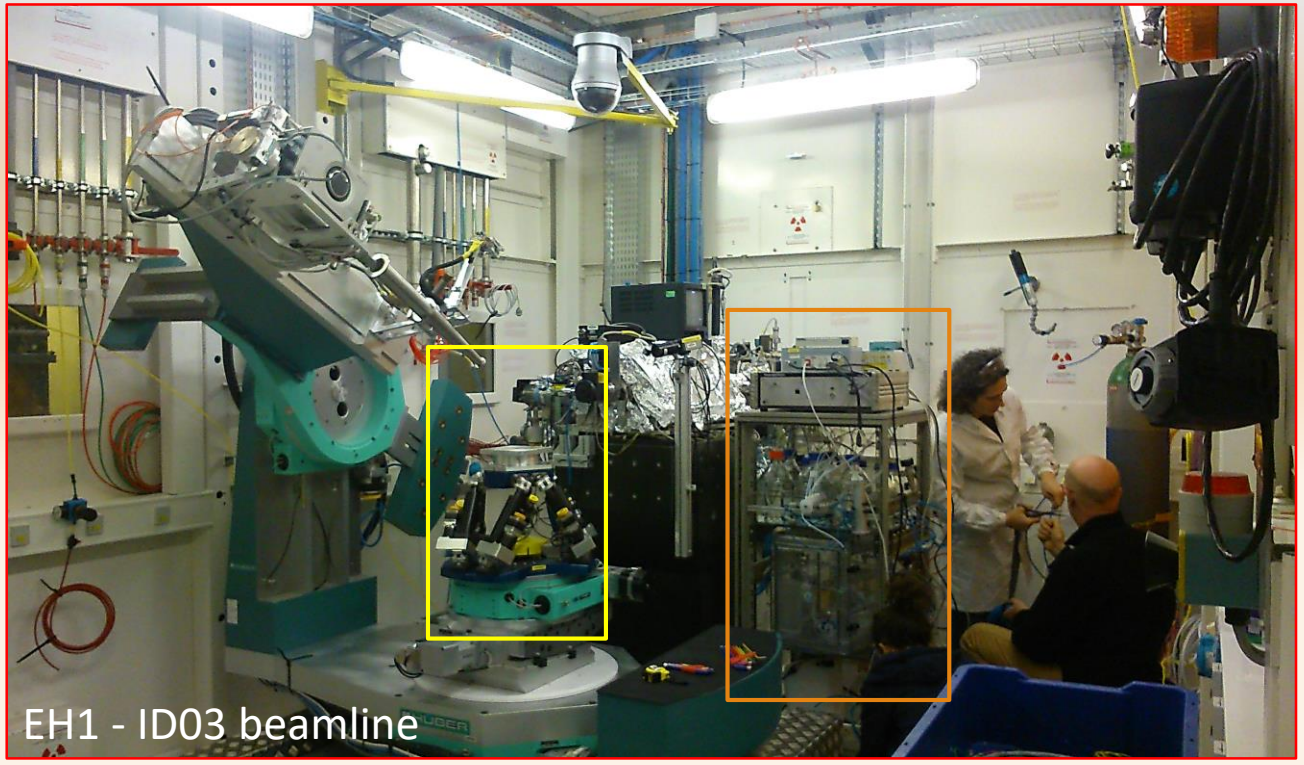


https://www.bloomberg.com/graphics/2015-whats-warming-the-world/

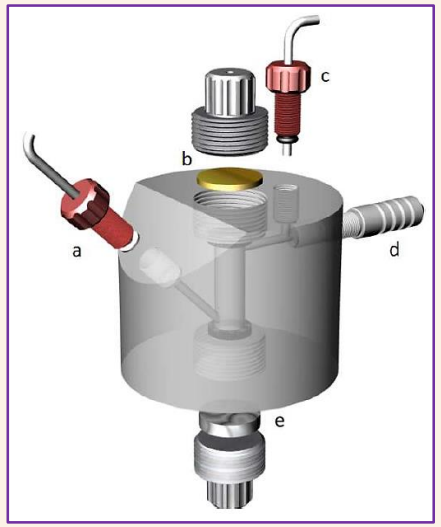
Best Research-Cell Efficiencies

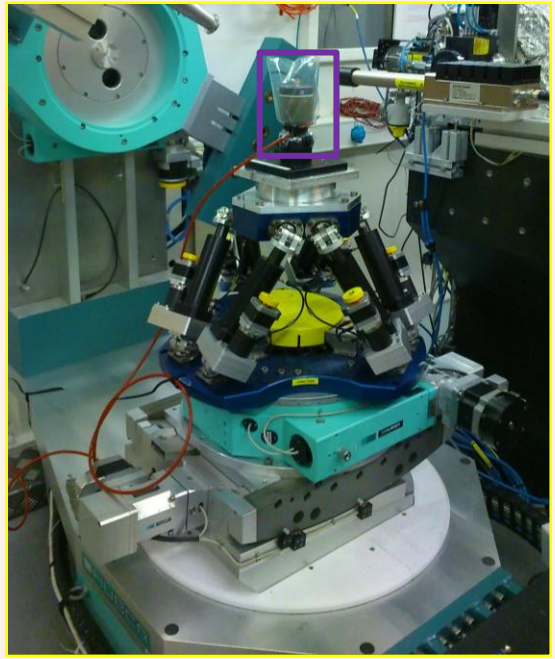


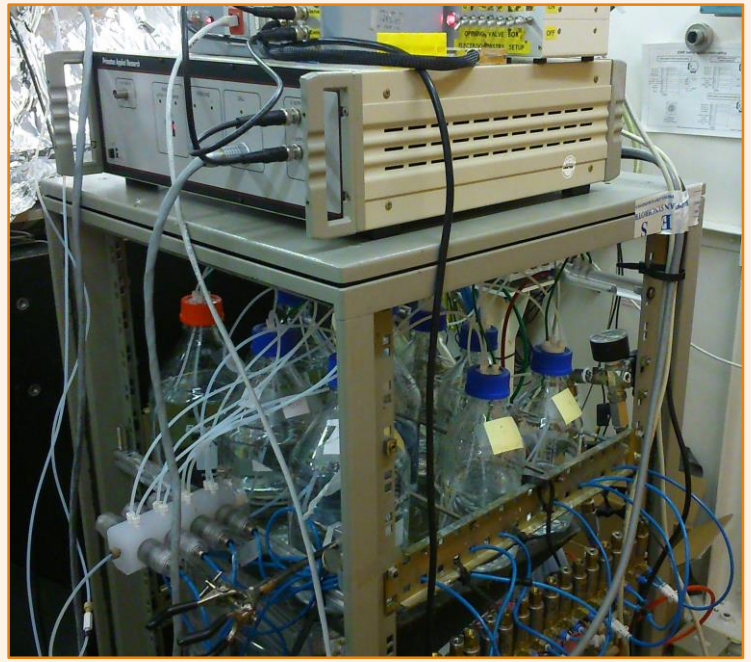
https://www.nrel.gov/pv/cell-efficiency.html



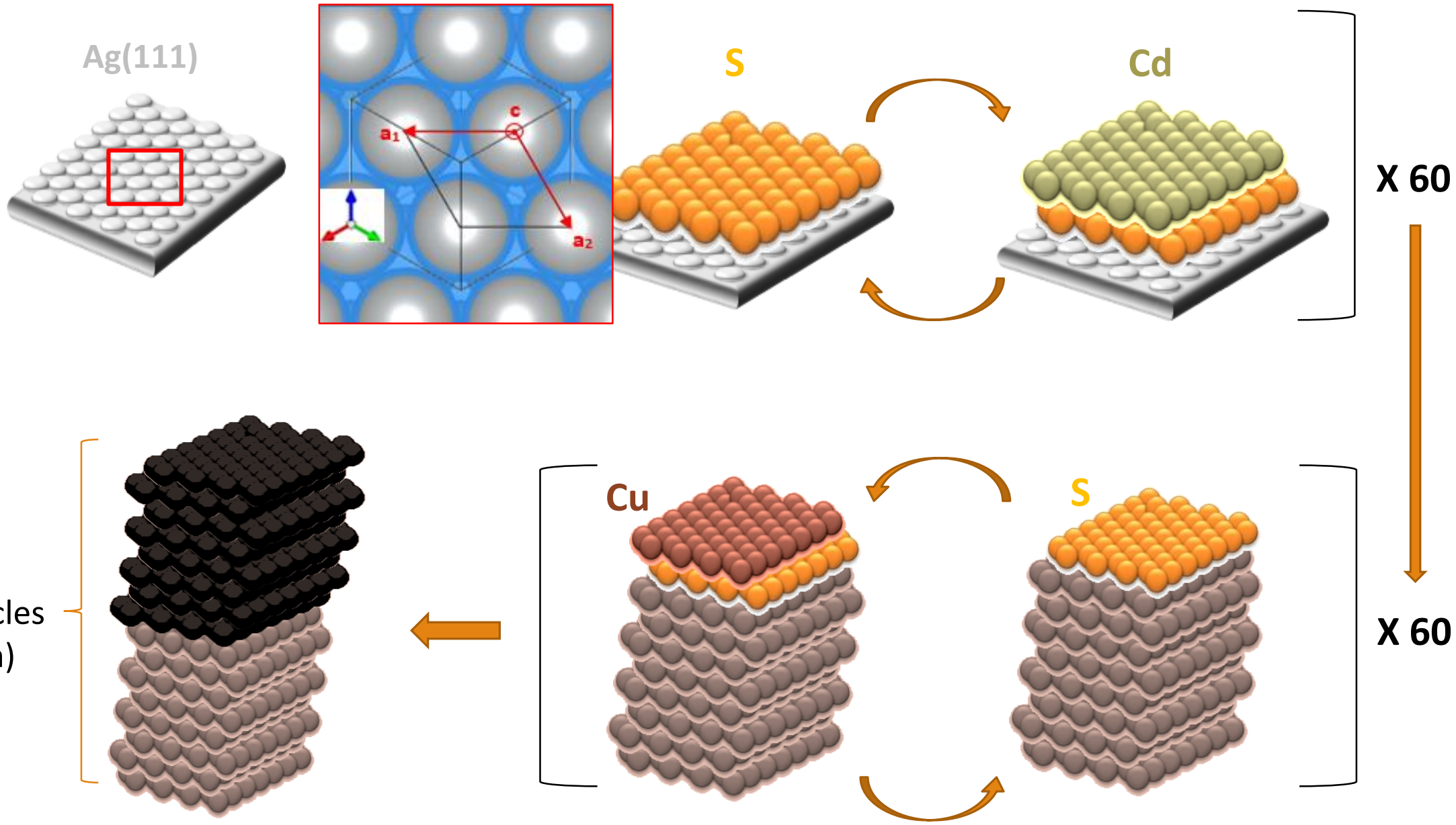
ESRF
The European Synchrotron



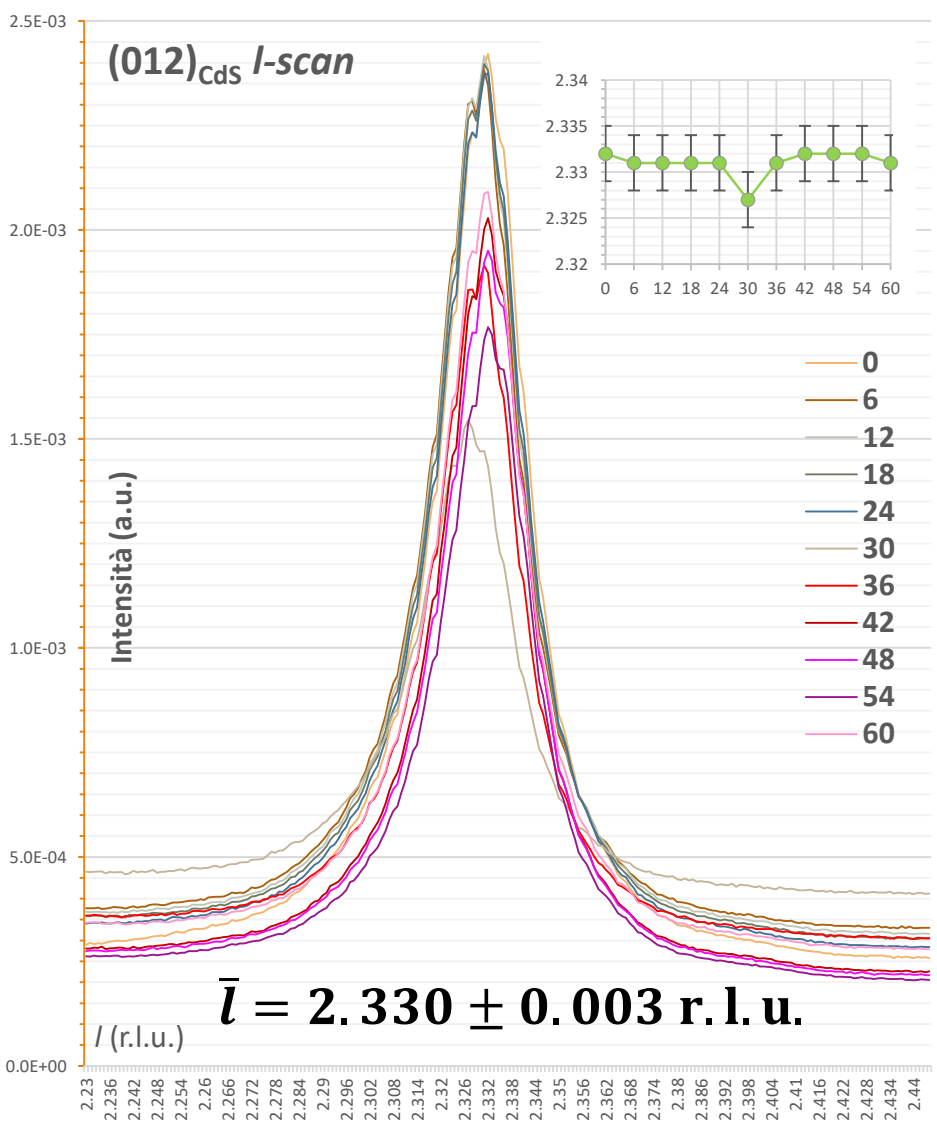


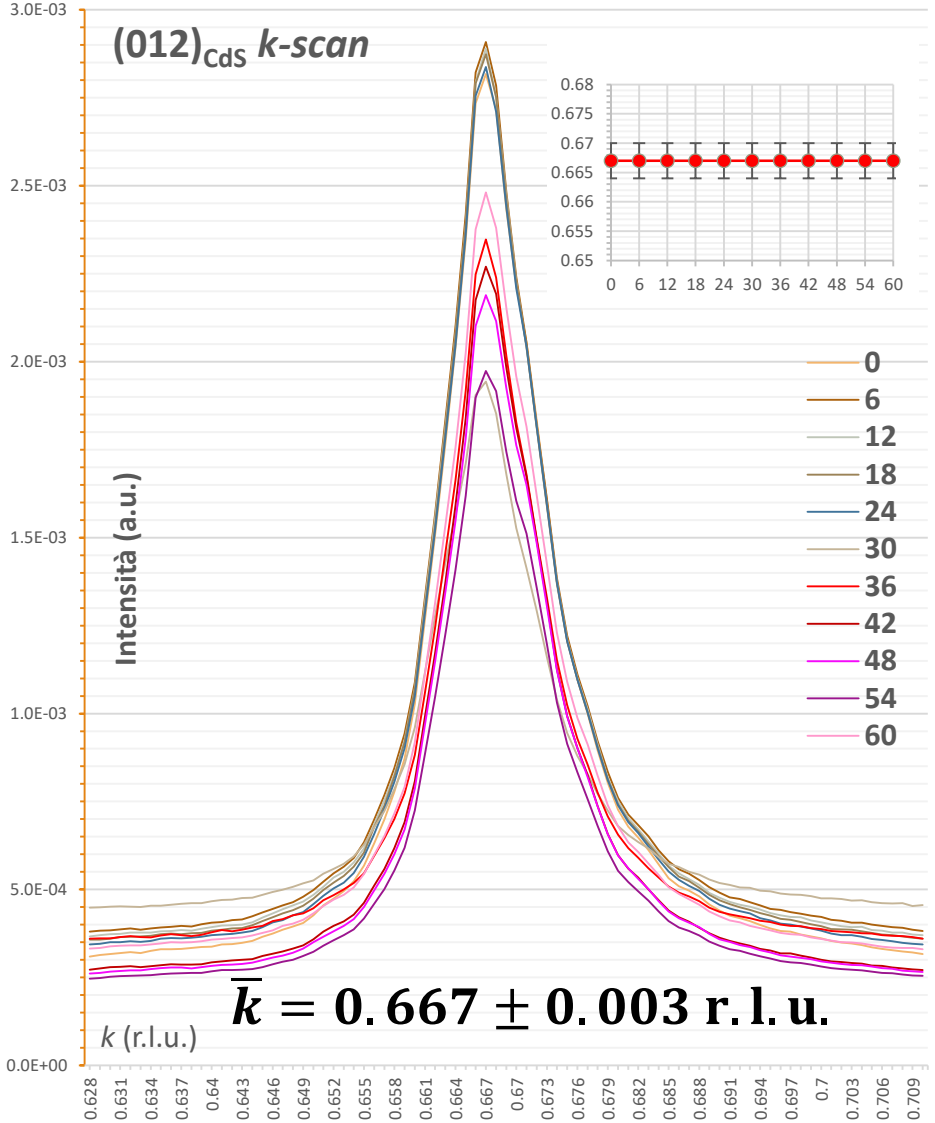


Sample preparation

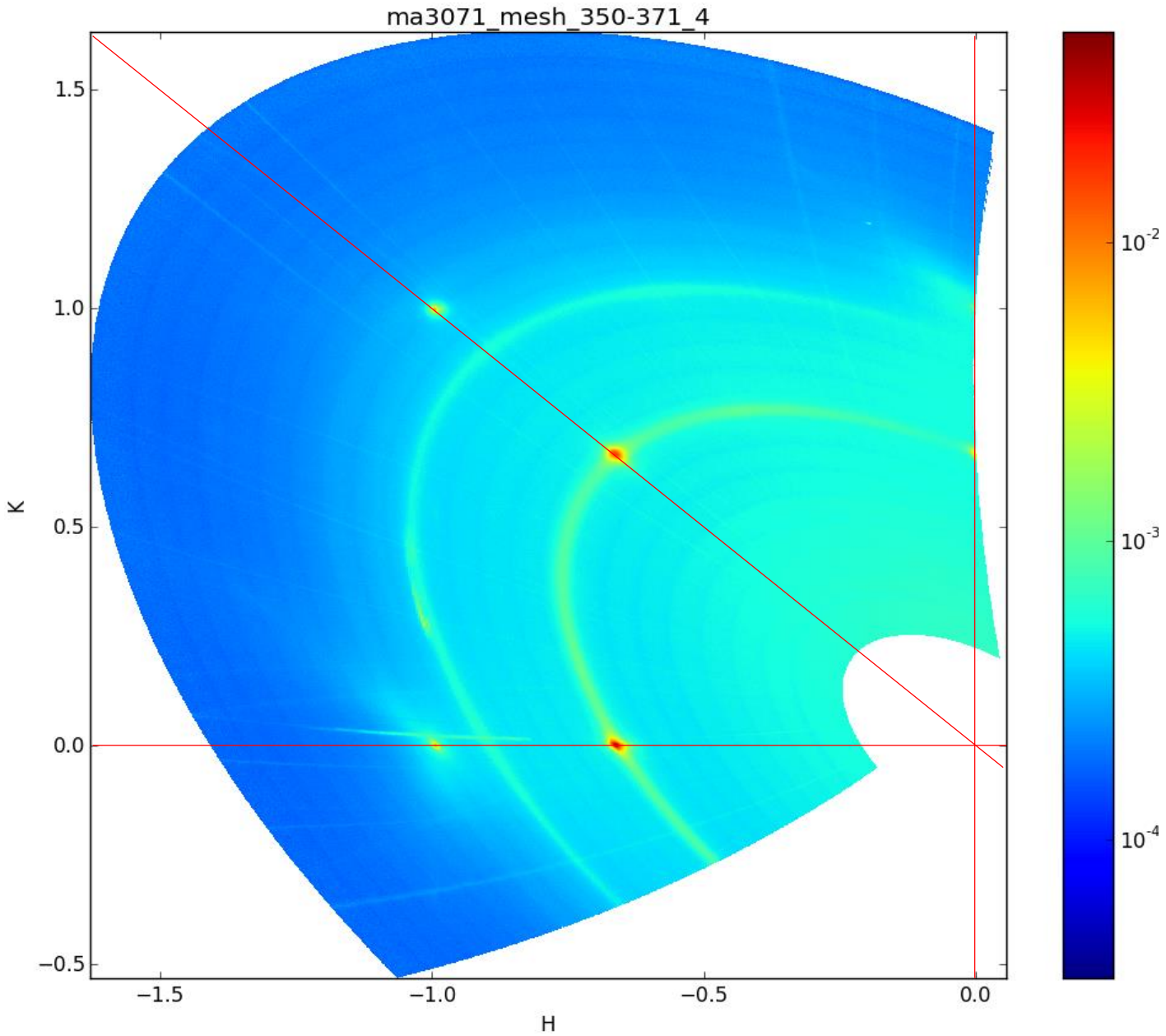


$(CdS)_{60}/Ag(111)$ structure vs N° Cu_2S cycle





$(CdS)_{60}$/Ag(111) 2-D BINoculars map



Greenockite

$P6_3mc$

$a = b = \mathbf{4.137}$ Å; $c = \mathbf{6.714}$ Å

$\alpha = \beta = 90°;\ \gamma = 120°$

$V = \mathbf{99.52}$ Å^3

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

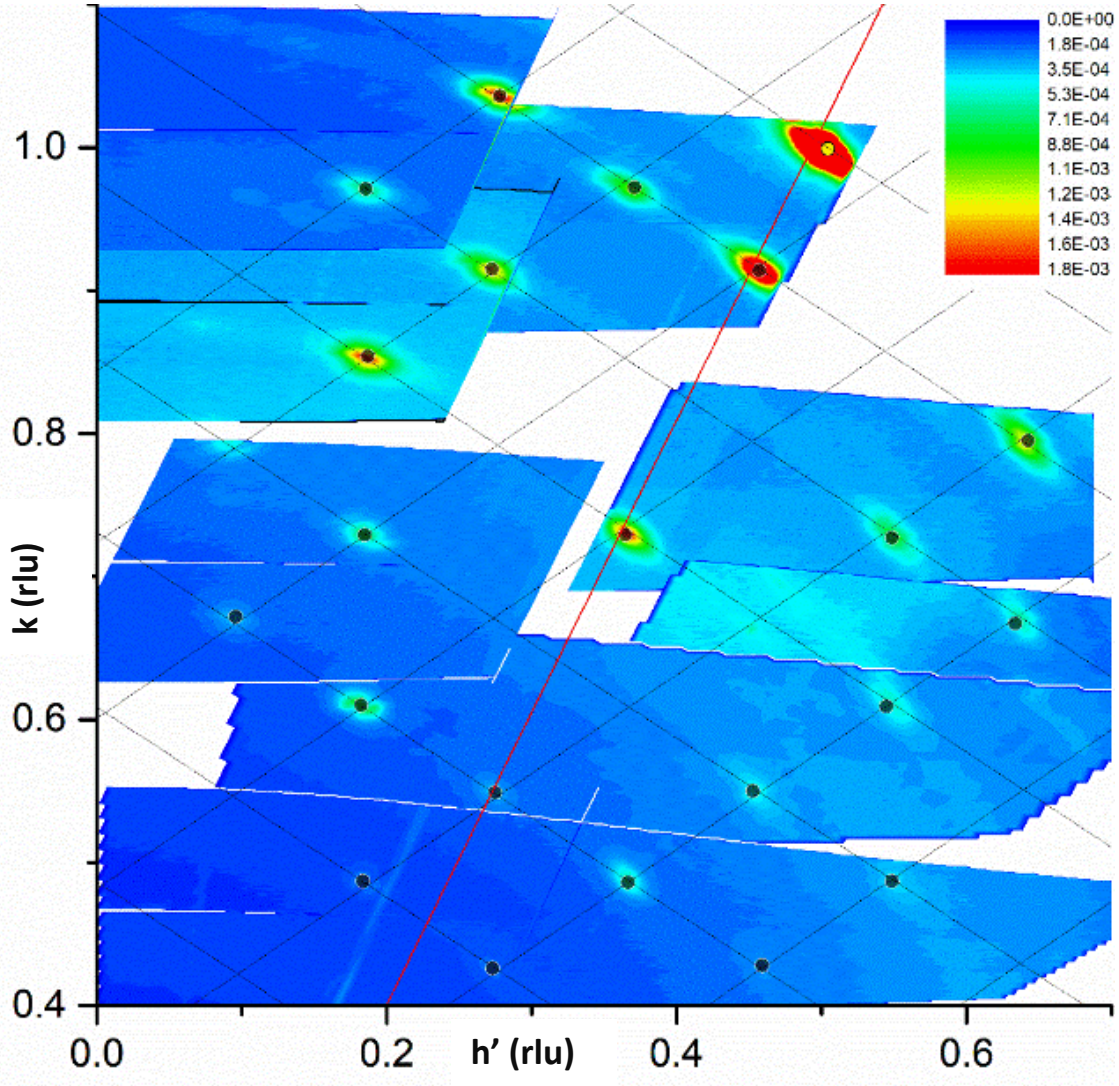
?

$a = b = \mathbf{4.332}$ Å; $c = \mathbf{6.075}$ Å

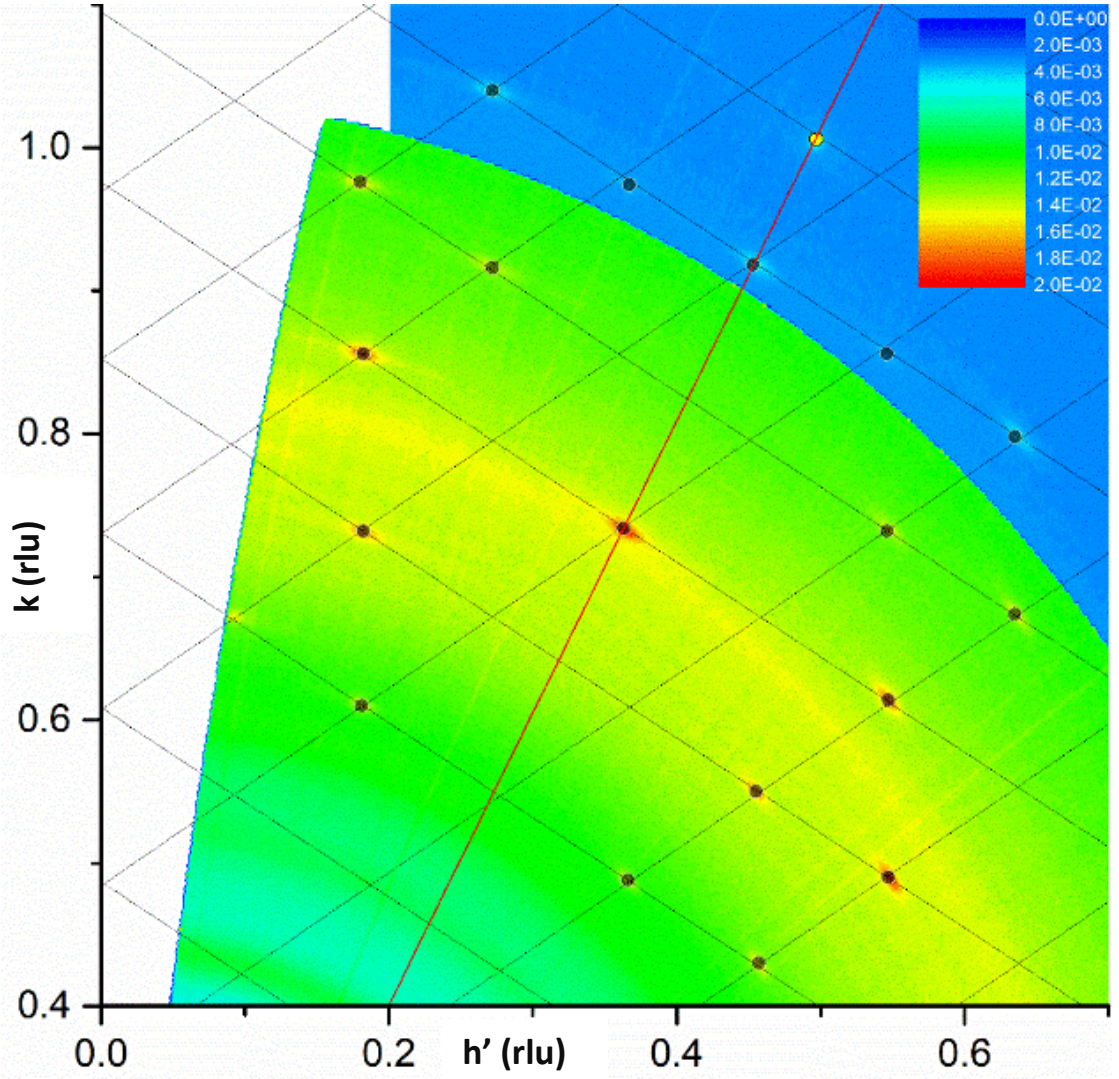
$\alpha = \beta = 90°;\ \gamma = 120°$

$V = \mathbf{98.73 \pm 0.37}$ Å^3

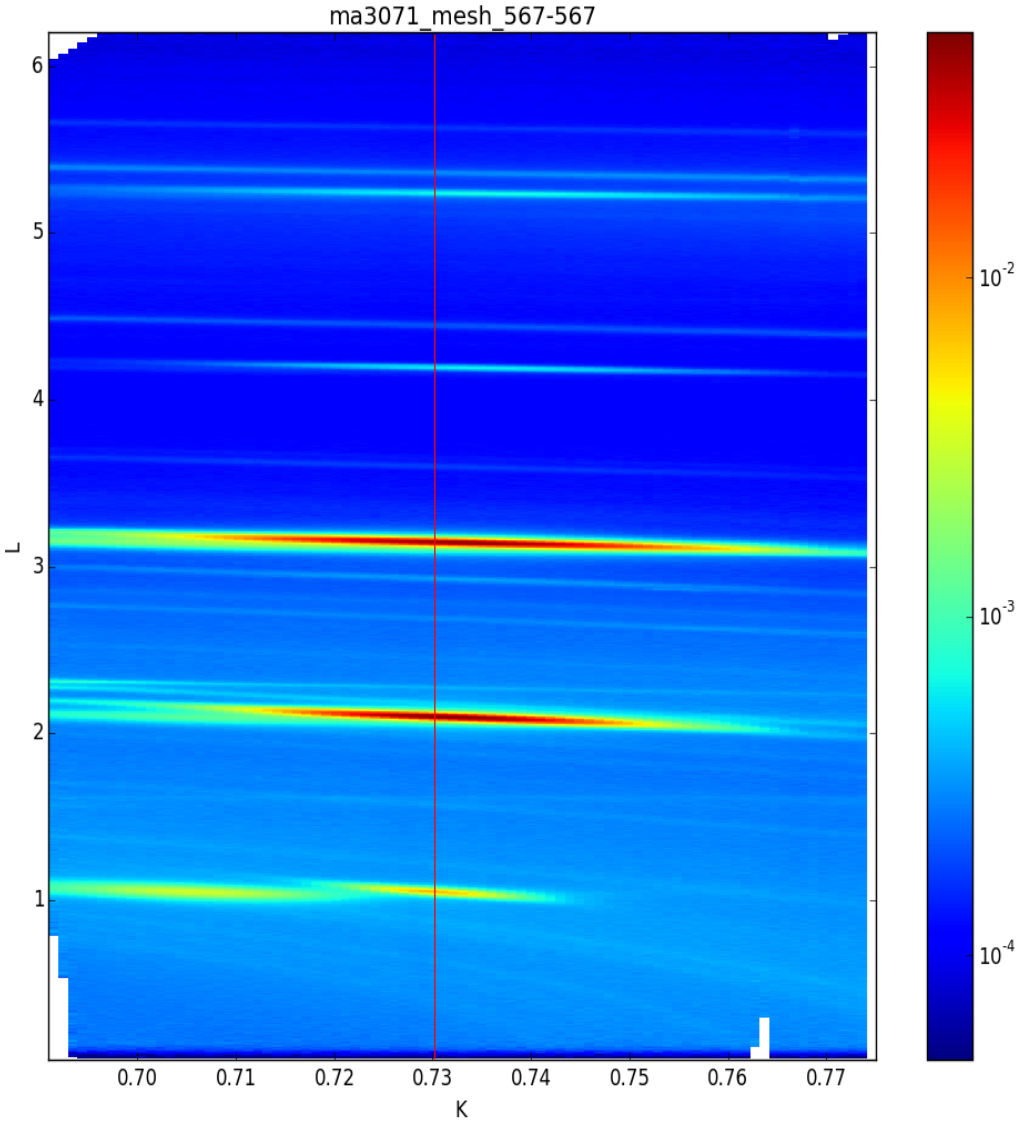
$(Cu_2S)_{60}/(CdS)_{60}/Ag(111)$
(MA3071)



$(Cu_2S)_{60}/Ag(111)$
(ma2082)



$(0\ 0.73\ 0.2\text{-}6)_{Cu_2S}$ *l-scan* and Cu_2S cell parameters



$(Cu_2S)_{60}/(CdS)_{60}/Ag(111)$

MA3071

$a = b = 27.41 \pm 0.04$ Å; $c = \boxed{6.76 \pm 0.03}$ Å

$\alpha = \beta = 90°;\ \gamma = 120°$

$c_{chalcocite} = 13.494$ Å

Conclusions

- MA3071 is the first *in-situ* SXRD experiment which features an E-ALD bi-layer junction of Cu_2S/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_2S 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_2S 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 chalcocite-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_2S/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.

1) Giaccherini et al. (2017), Scientific Reports | 7: 1615 | DOI:10.1038/s41598-017-01717-0