Charge Transport Mechanism in Cu_2O

Way to find out its low performance in solar cells

Garima Aggarwal, PhD

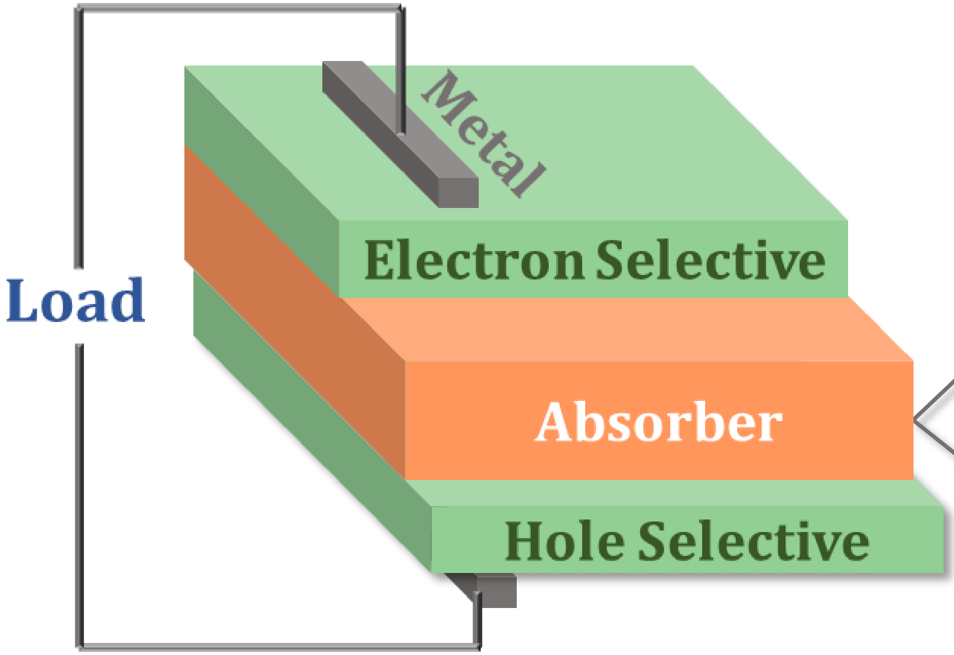
Supervisor: Prof. K. R. Balasubramaniam

Energy Science & Engineering Department

Indian Institute of Technology Bombay India

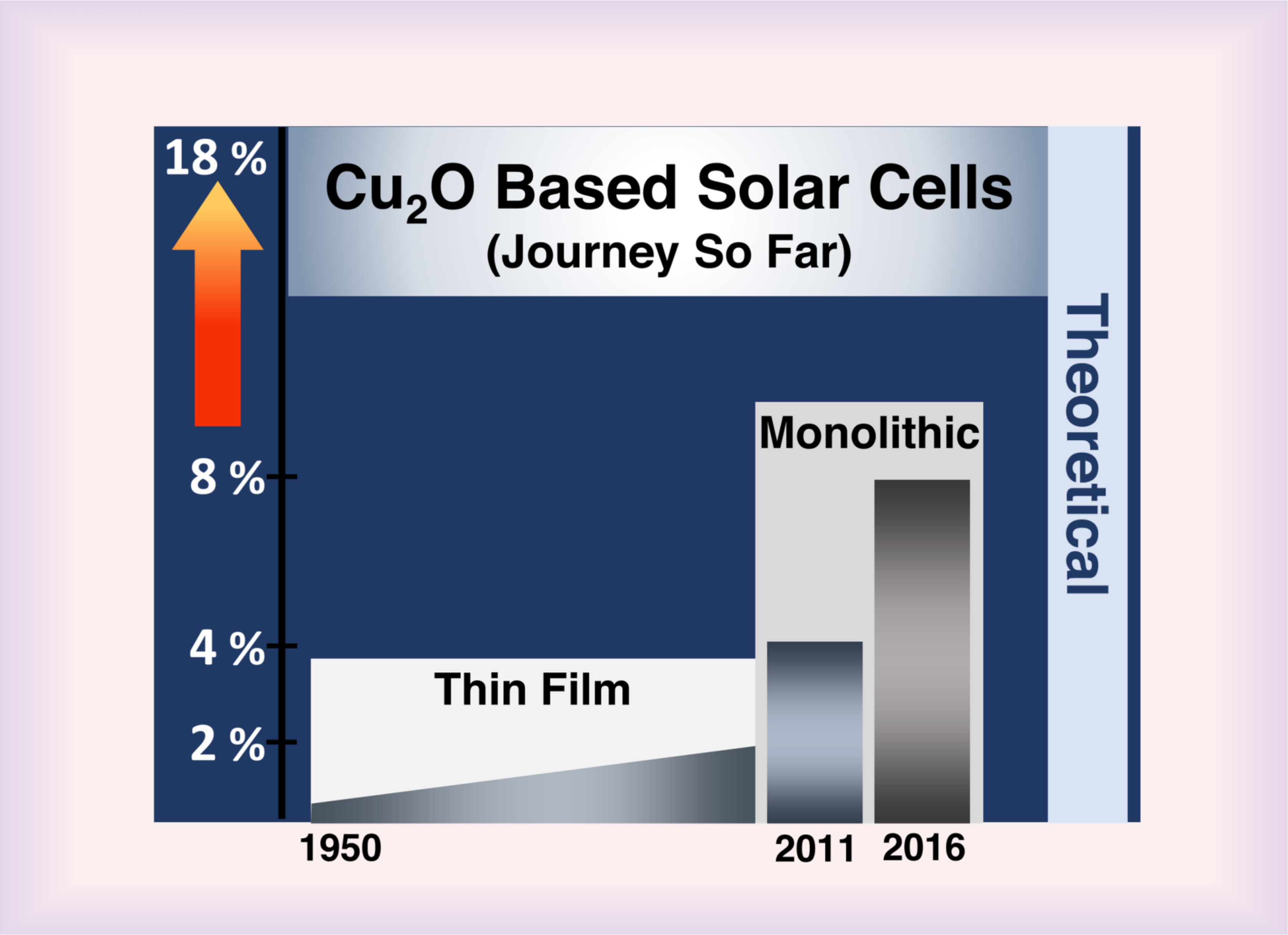
Solar Photovoltaic Cell Structure & Materials

Light Absorption → e-h pair Generation → Separate collection of charge carriers → Transfer to external circuit



- Silicon (single/multi-junction)
- Chalcogenides (CIGS, CZTS)
- Dye-senstitized
- Perovskite (organic/inorganic)
- Metal Oxides

Abundance | Processing Cost | Toxicity | Optical/Electrical Properties



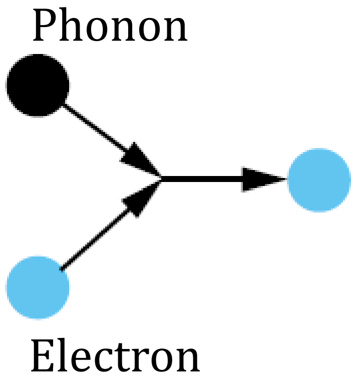
18 %
Cu_2O Based Solar Cells
(Journey So Far)
Theoretical
Monolithic
8 %
4 %
Thin Film
2 %
1950
2011
2016

Optical & Electrical Properties of Absorber Layer

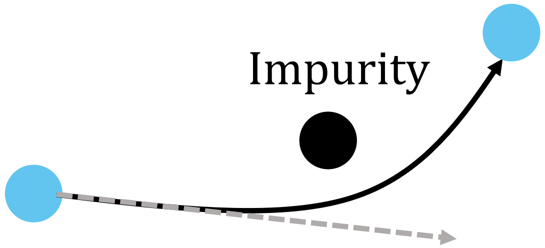
Cu_2O

Abundant, easy processing

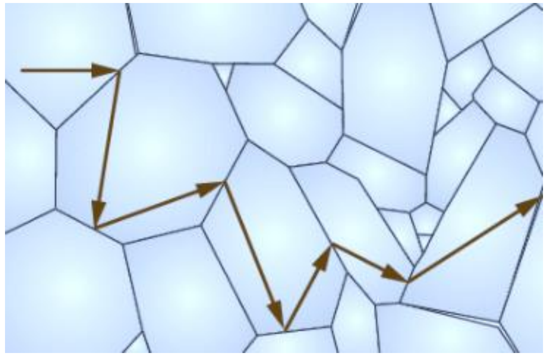
- Direct bandgap ✓
- High absorption co-efficient ✓
- Charge carrier mobility ↓



Phonon Scattering



Ionized/neutral Impurity Scattering



Grain Boundary Scattering

Dominant Scattering in Cu_2O at RT is still not clear

Objective

Explore the effects of

Microstructural properties

Grain boundary type

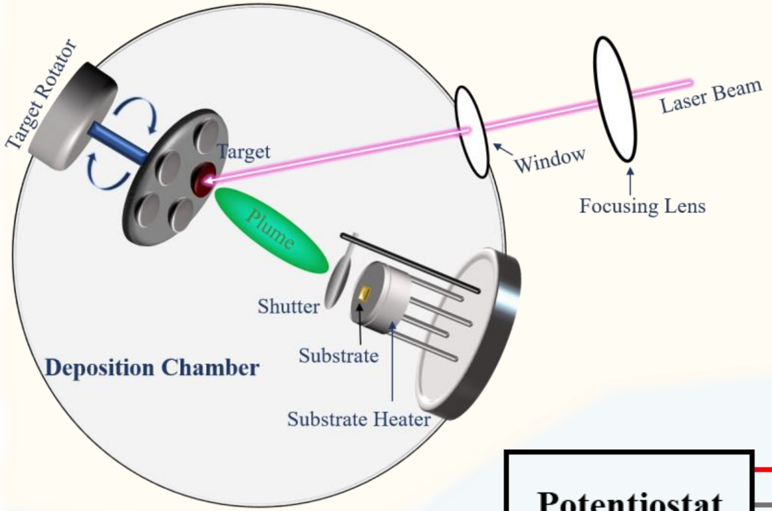
Grain boundary cross-section

and *Charge defects*

on

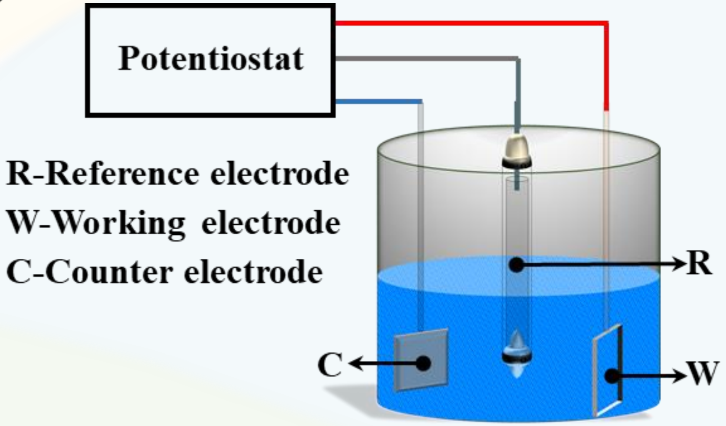
Hole transport in Cu_2O

Strategy: Synthesize an array of samples



Pulsed Laser Deposition

- Epitaxial growth of Cu_2O on crystalline LSAT substrates
- Textured, low angle grain boundaries

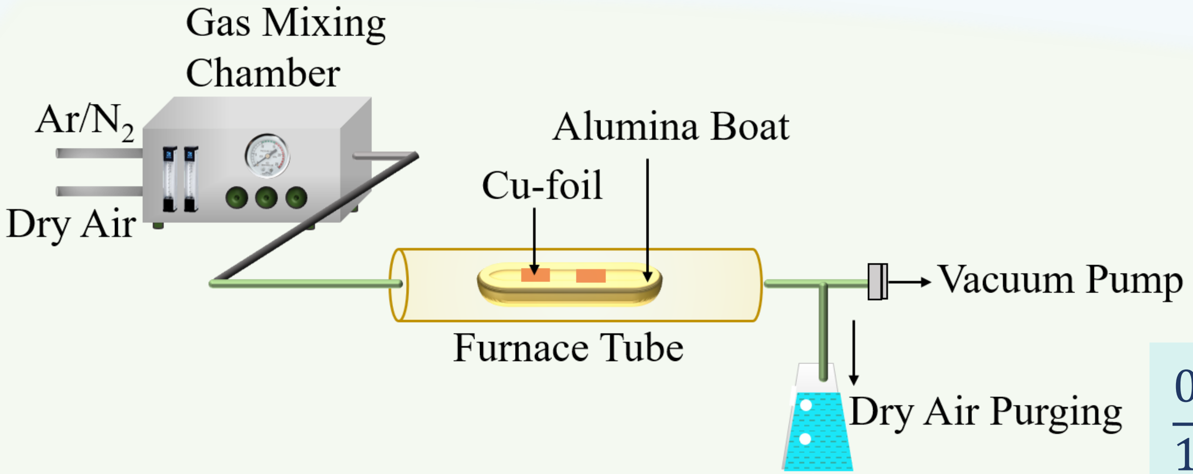


Electrodeposition

- Patterning of metallic substrate and continuous film on top
- Textured, high angle grain boundaries

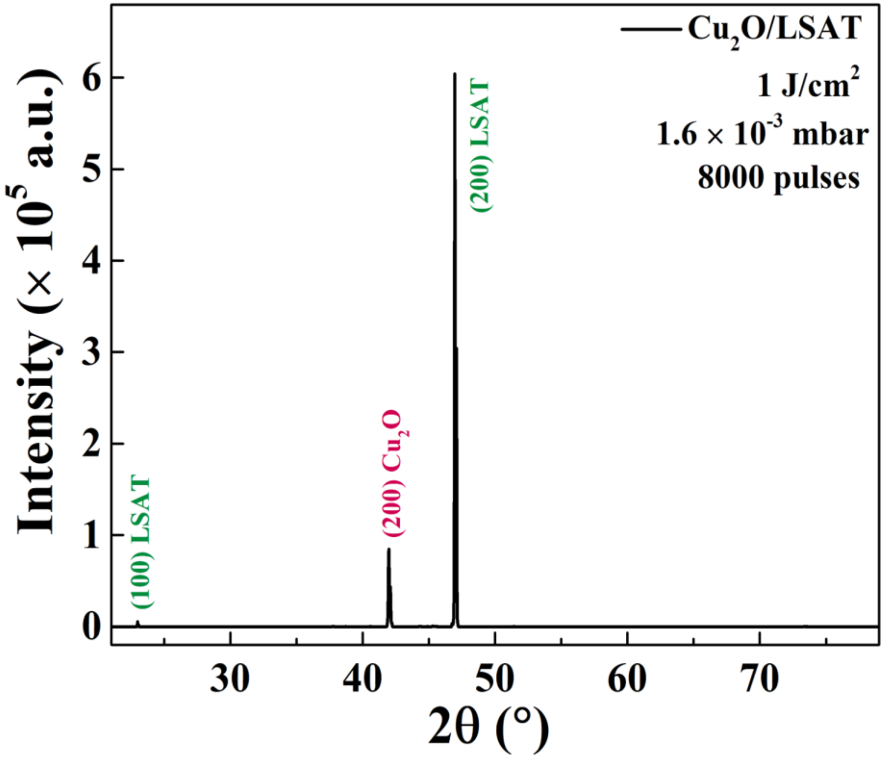
Thermal Oxidation

- Thorough grain growth study to obtain variable grain size
- Produced single crystal samples of size 1 cm
- Polycrystalline, high angle grain boundaries

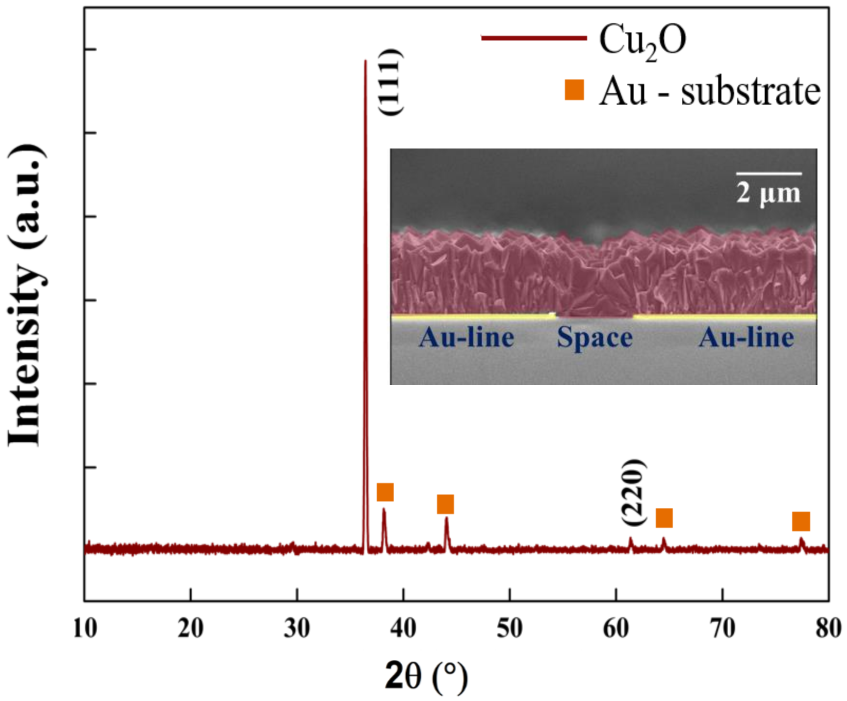


Grain Boundary Characteristics

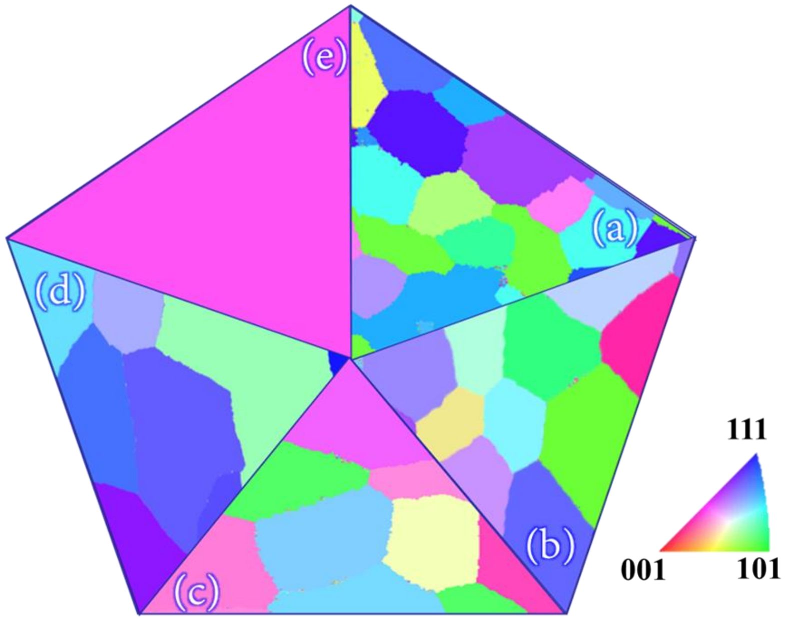
Pulsed Laser Deposition



Electrodeposition



Thermal Oxidation



- Phase pure (100) textured Cu_2O
- Low angle grain boundaries
- $\{001\}_{Cu_2O} | \{001\}_{LSAT} || < 110 >_{Cu_2O} | < 110 >_{LSAT}$

- Phase pure (111) textured Cu_2O
- High angle GB
- Cu_2O film on patterned-Au

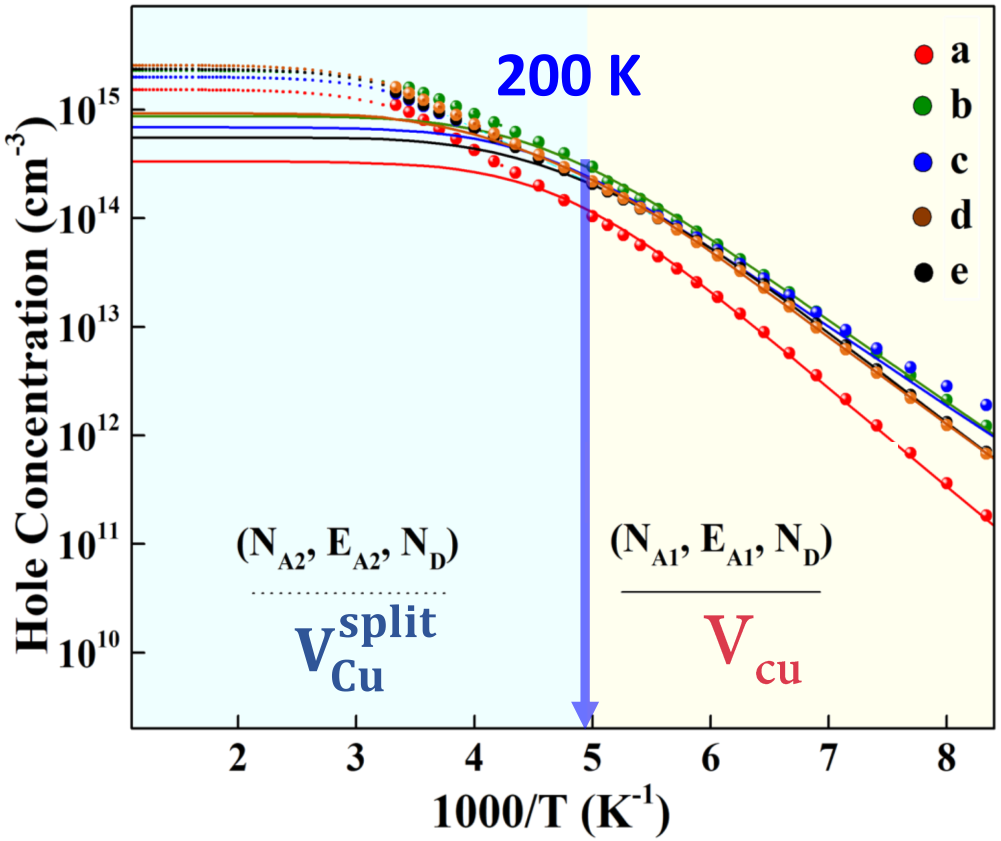
- Phase pure polycrystalline Cu_2O
- High angle GB
- Variable grain size

Charge carrier transport mechanism

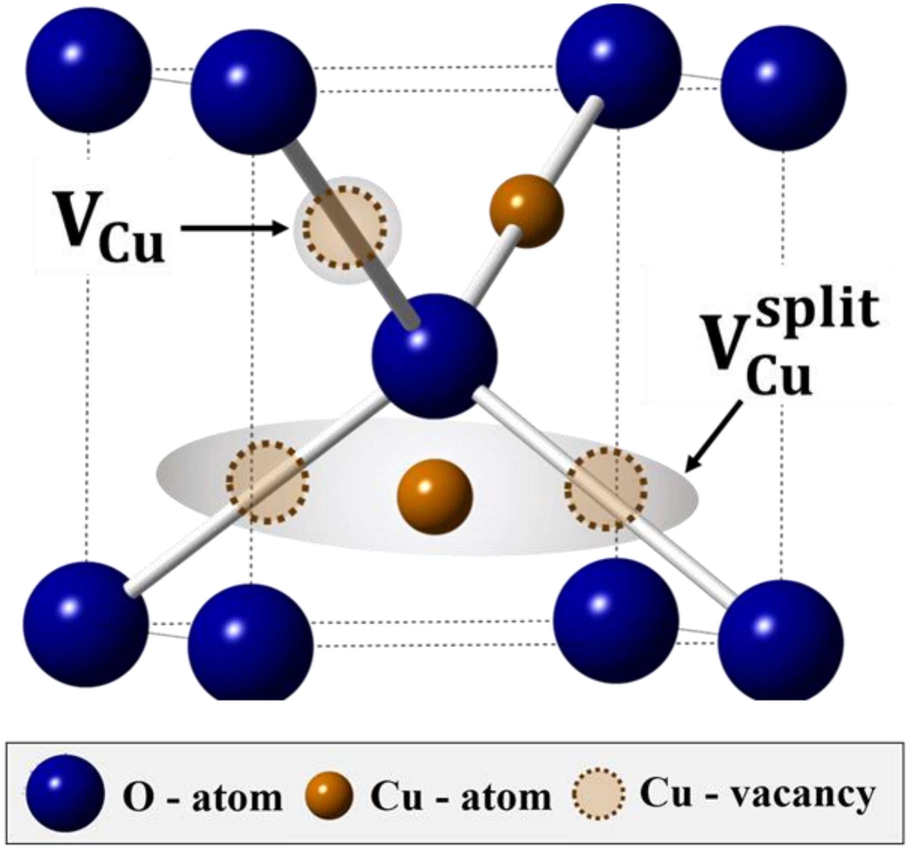
1. Information of Intrinsic Charged Defects

2. Dominant Carrier Scattering Mechanism

Presence of Charged Point Defects/Clusters



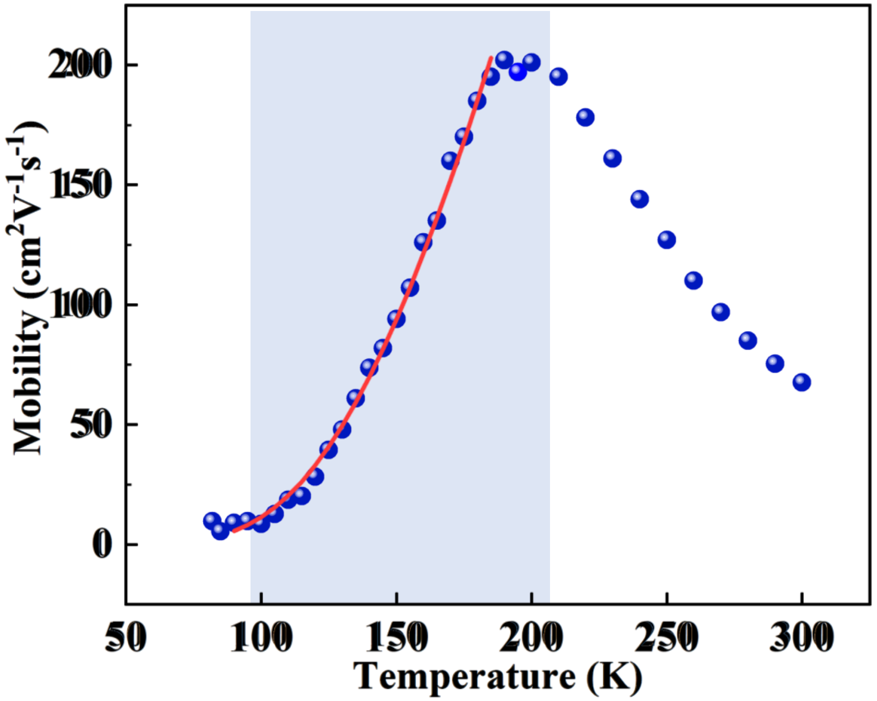
Two acceptor – one donor model



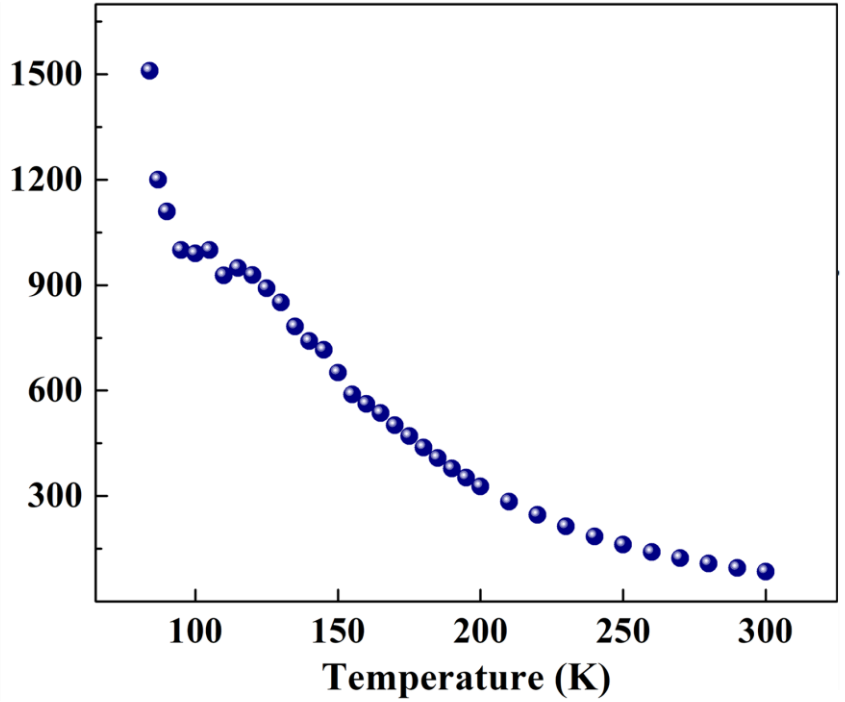
- There are two ionized acceptor type of defects present in Cu_2O at RT
- The defect cluster is dominant at T > 200 K

Dominant Carrier Scattering Mechanism (Low-T mobility)

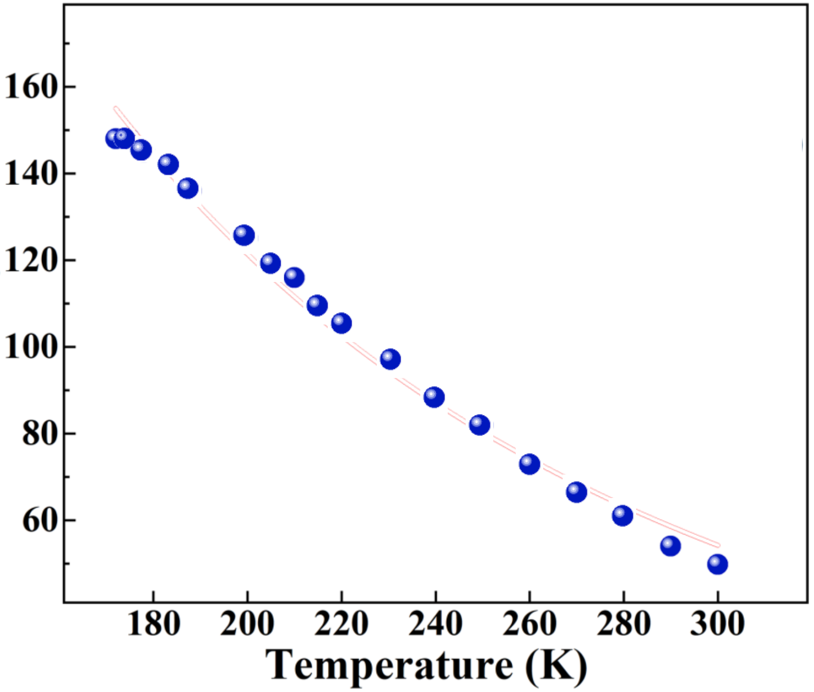
Poly-crystalline Sample - TO



Single Crystal Sample - TO



Low angle GB - PLD



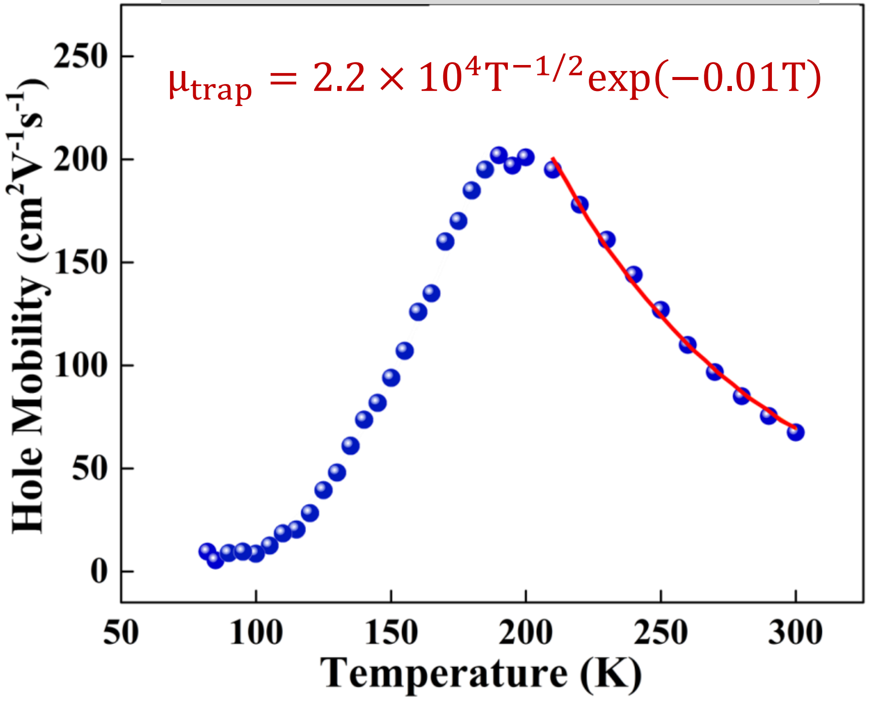
Low Temperature mobility (GB)

$$\mu_{GB} = AT^{-1/2}\exp\left(\frac{-\varphi}{KT}\right)$$

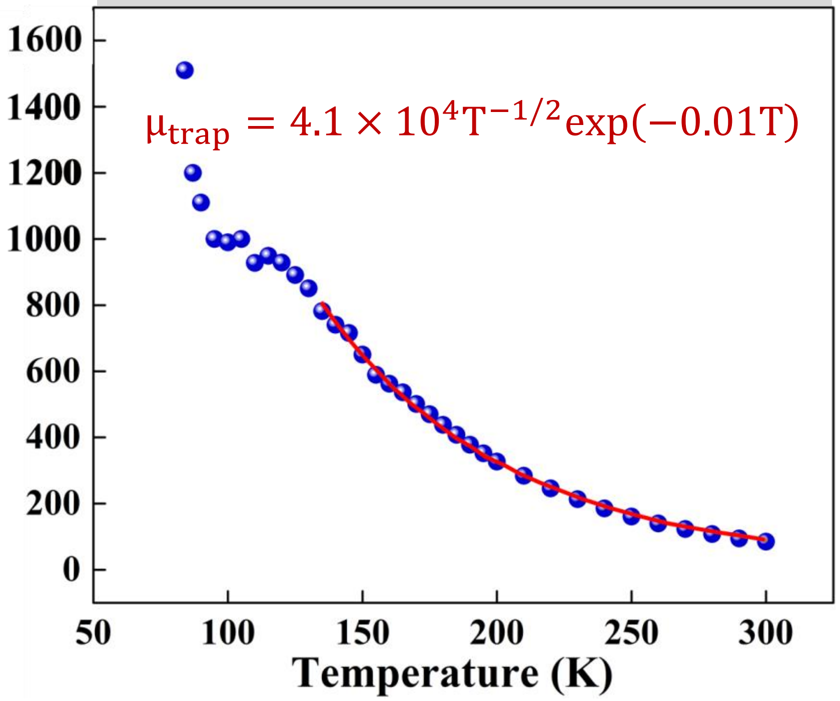
- GB scattering mechanism is dominant at T < 200 K
- Low angle GB's do not affect the charge transport

Dominant Carrier Scattering Mechanism (High-T mobility)

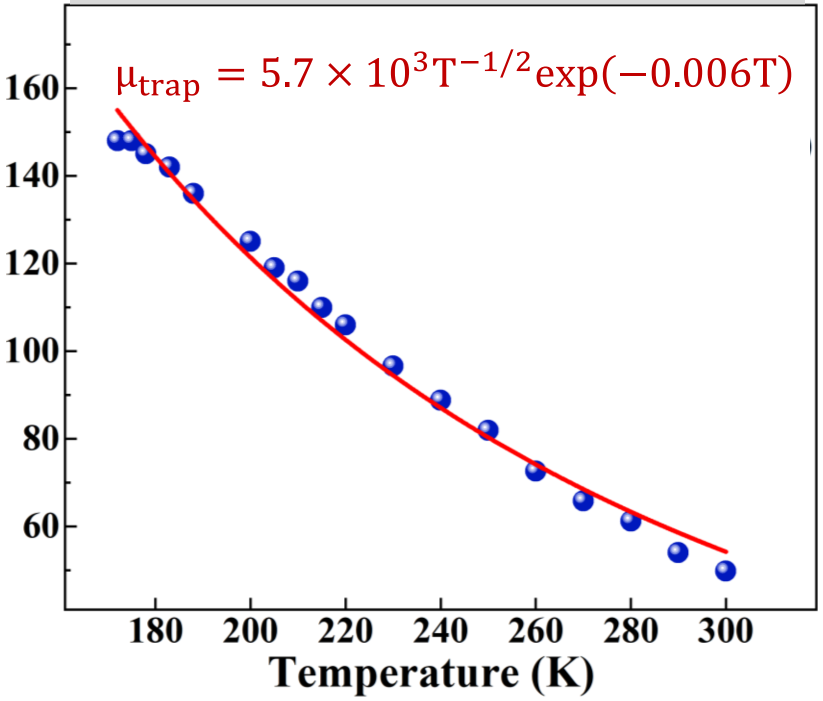
Poly-crystalline Sample-TO



Single Crystal Sample-TO



Low angle GB - PLD



High T mobility (Trap)

$$\mu_{trap} = BT^{-1/2} \exp(-CT)$$

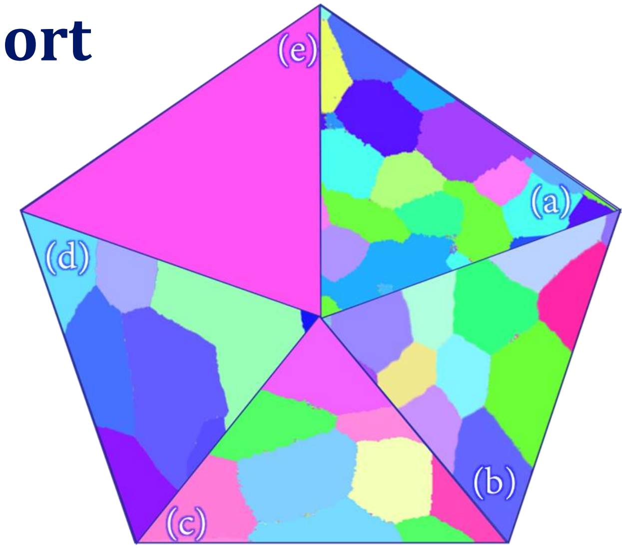
Proposed mechanism

- Capture cross-section of trap increases exponentially with T
- V_{Cu}^{split} works as a trap centre

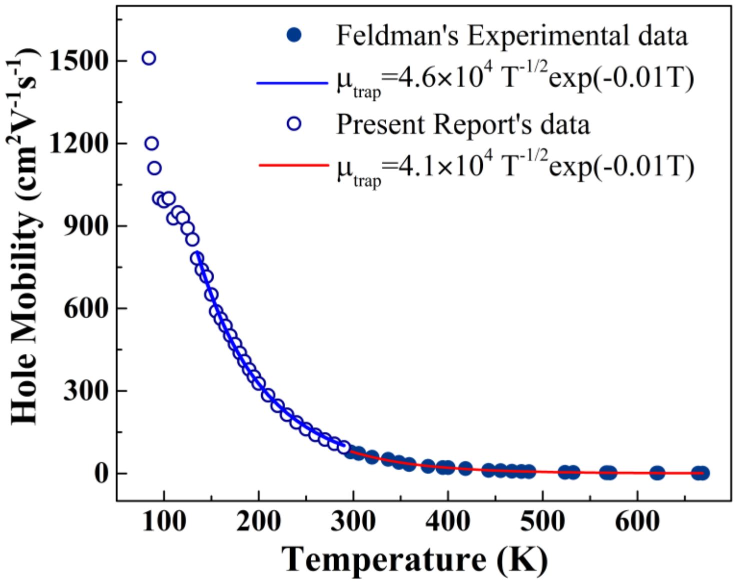
- Trap mediated scattering mechanism at T > 200 K

Conclusions

◇ **Microstructural characteristics do not influence RT hole transport**



◇ **Intrinsic defects determine μ_{RT}**



◇ **Instead of single crystal, device architecture,**

We need to focus on <u>Intrinsic Defect Neutralization</u>

Journal Articles from this work

- **G. Aggarwal,** A. J. Singh, H. K. Mehtani, K.R. Balasubramaniam, Strain induced abnormal grain growth in thermally oxidized Cu_2O sheets, Applied Physics Express, 14(3), 035503, 2021.
- **G. Aggarwal**, S. K. Maurya, A. K. Singh, K. R. Balasubramaniam, Intrinsic acceptor-like defects and their effect on carrier transport in polycrystalline Cu_2O photocathodes, Journal of Physical Chemistry C, 123(43):26057-26064, 2019.
- **G. Aggarwal**, C. Das, S. Agarwal, S. K. Maurya, P. R. Nair, K.R. Balasubramaniam, Hall mobility of as-grown Cu_2O thin films obtained via electrodeposition on patterned Au substrates, Physica Status Solidi RRL, 12(1):1700312, 2018.
- **G. Aggarwal**, Nawaf A, A. J. Singh, Dayadeep Monder, K.R. Balasubramaniam, Defect-dopant association in Cu_2O: Presence of triple acceptors. (Under Review in Physical Review B)

Conference Presentations

- **G. Aggarwal**, S. K. Maurya, and K. R. Balasubramaniam, *American Physical Society (APS) March Meeting 2020*
- **G. Aggarwal**, S. K. Maurya, and K. R. Balasubramaniam, *American Physical Society (APS) March Meeting 2019*
- **G. Aggarwal**, Ashish K. Singh, S. K. Maurya, and K. R. Balasubramaniam, *International Conference on Advances in Energy Research (ICAER) 2017* **(Published in proceedings as: *Advances in Energy Research*, Vol. 1 (pp. 191-197), 2020)**
- **G. Aggarwal**,S. K. Maurya, and K. R. Balasubramaniam, *Material Research Society (MRS) Fall Meeting 2017*

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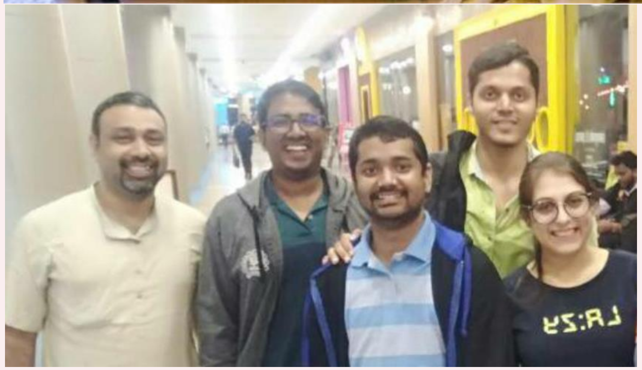

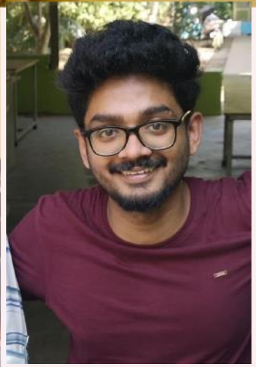

Energy Materials Synthesis Lab

Department of Energy Science and Engineering

Indian Institute of Technology Bombay

Thank you
&
Questions

Email id: garima.agrawalsk@gmail.com

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