Transparent Conducting Oxide Electrodes

Grain boundary scattering in undoped and doped In_2O_3

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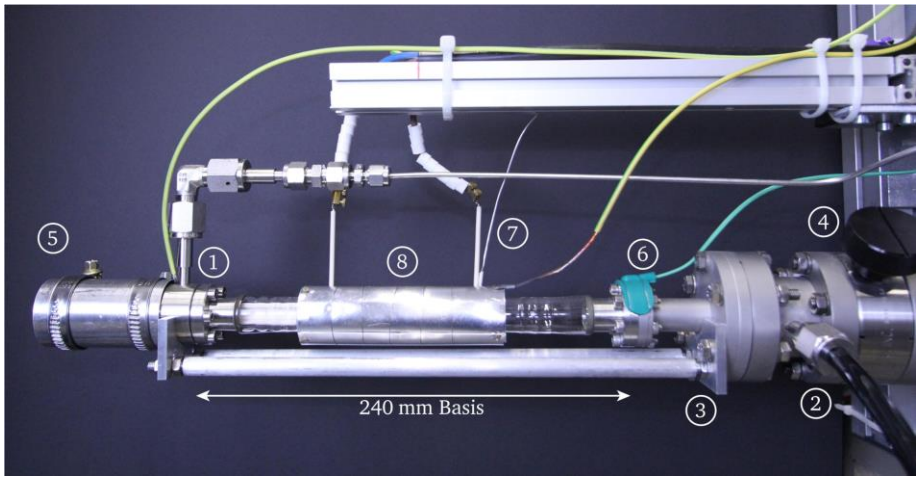

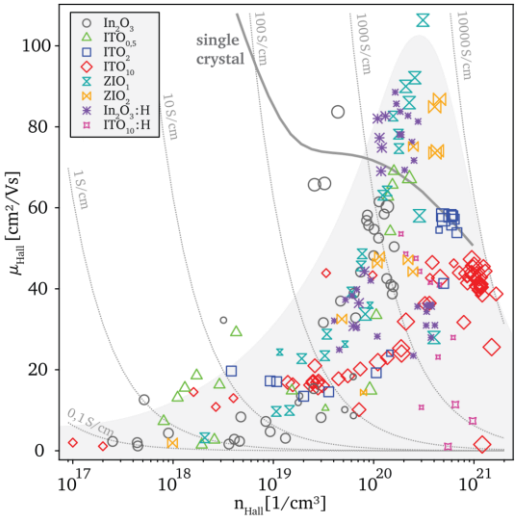

Motivation: The TCO electrode for organics

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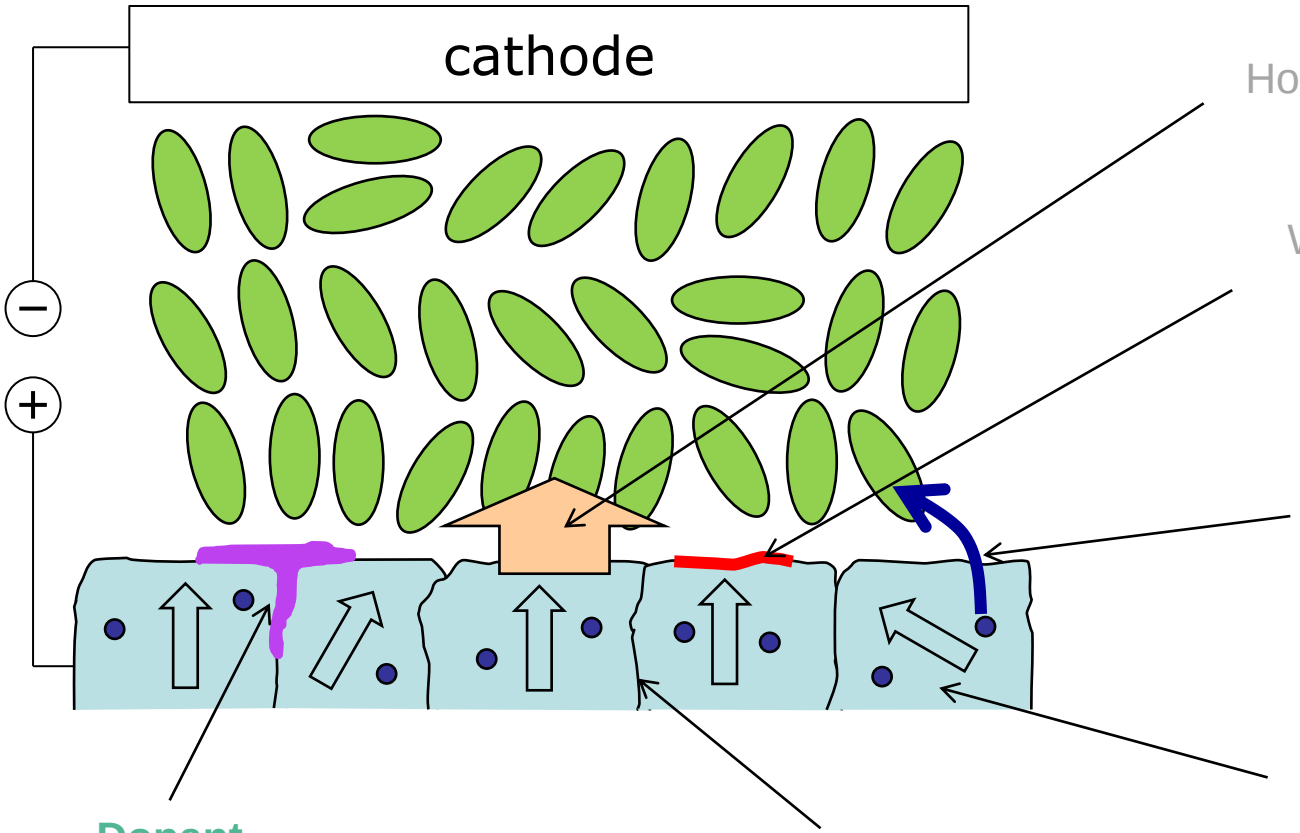

Hole injection determined by work function

Work function determined by surface orientation and termination

Oxygen exchange (relaxation measurements)

Conductivity σ depends on carrier concentration *n* and mobility *μ*

$$\sigma = en\mu$$

Dopant segregation

Mobility *μ* determined by material properties (grain boundaries) and doping elements

$p(O_2)$ dependent Hall-relaxation measurement of undoped In_2O_3

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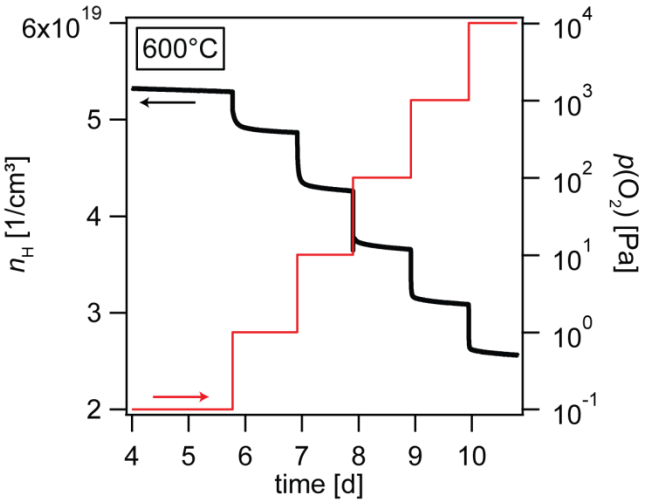
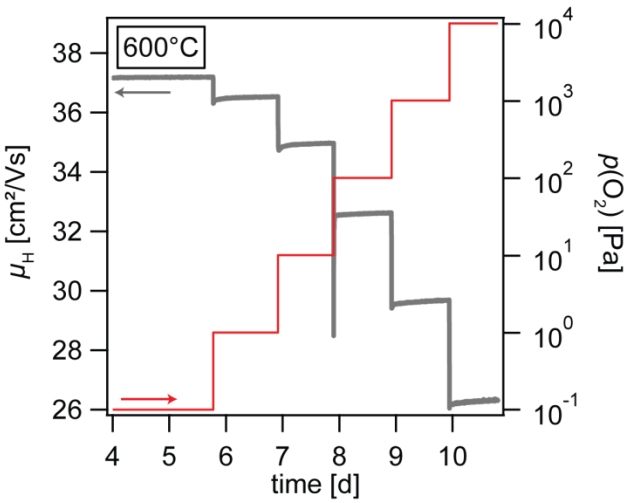
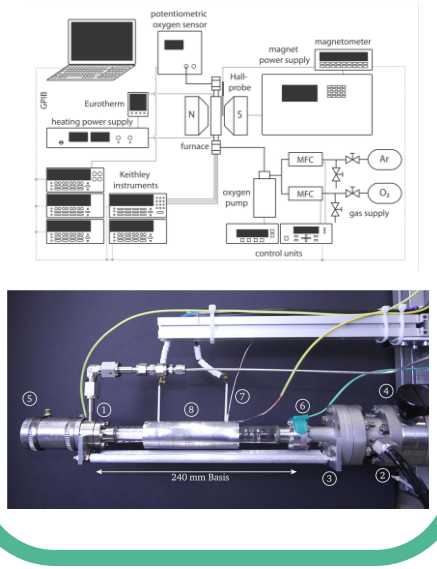
Carrier concentration

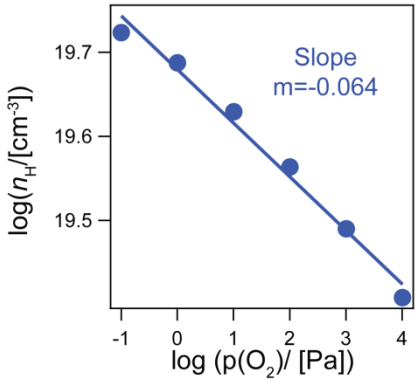


Carrier mobility



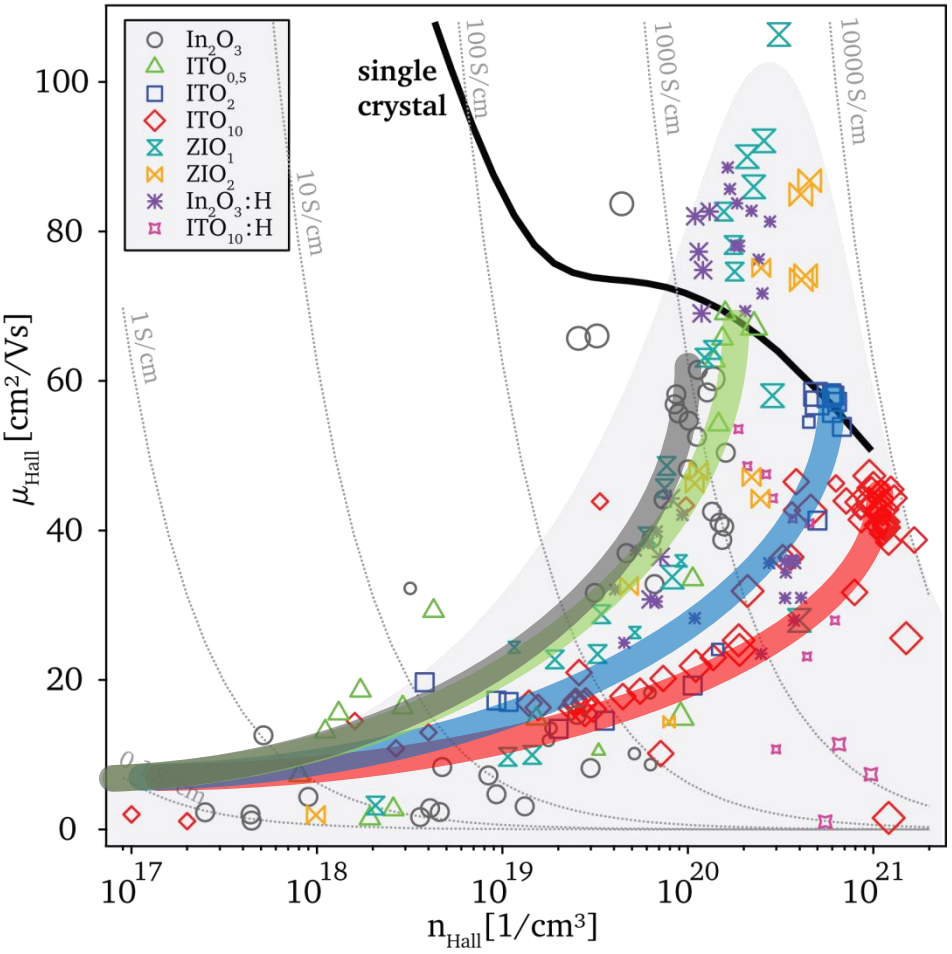
Setup





- *Carrier concentration n* changes reversibly with oxygen partial pressure
  - ➢ Slope of Brouwer plot does not correspond to expected $p(O_2)^{-1/6}$ dependence
- *Carrier mobility μ* also depends on oxygen partial pressure:
  - ➢ due to changes in carrier concentration and changes in **grain boundary barrier** ???

Influence of doping elements on In_2O_3



Element	Short	Concentr.	Purpose
Sn	ITO	0.5, 2, 10 wt% SnO_2	Most used, Segregation effects?
Zr	ZIO	1, 2 wt% ZrO_2	High mobility
H	In_2O_3:H		High mobility, low processing T

Scattering mechanisms in In_2O_3 :

- Phonon Scattering
- Ionized Impurity Scattering
- Grainboundary Scattering

} Single crystal (O. Bierwagen)

For $n < 10^{20}$ 1/cm³ μ is decreasing:

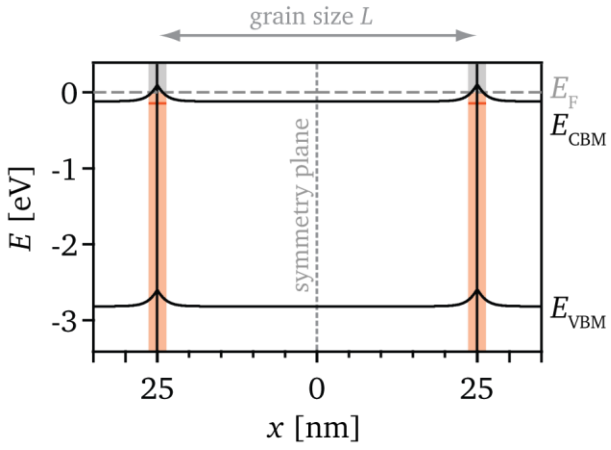
➢ effect of grainboundary scattering

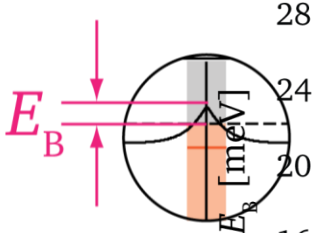
Different dopings behave differently

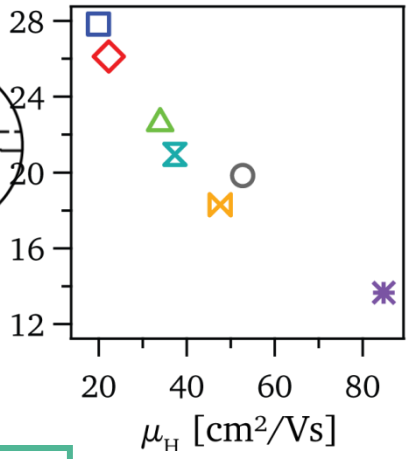
➢ Segregation at grain boundaries?

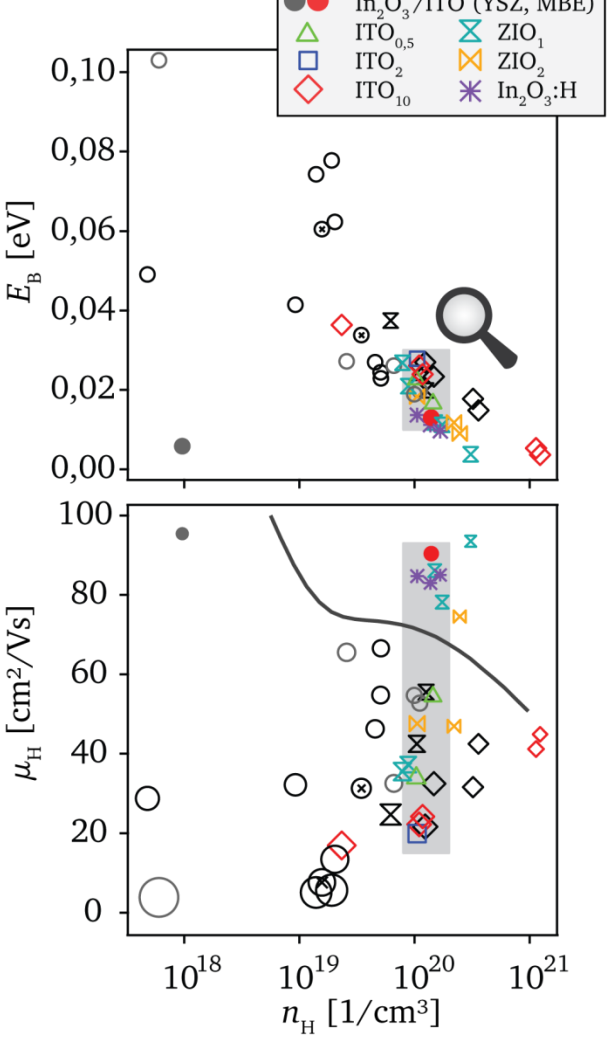
Cooperation with O. Bierwagen, Paul-Drude-Institut, Berlin

GB Scattering – measured barriers









$$\mu_{GB}(T) = \mu_{0,300\,K} \cdot \left(\frac{T}{300\,K}\right)^{-\beta} \cdot \exp\left(-\frac{E_B}{k_B T}\right)$$

Barriers E_B…
- were successfully measured
- increase with decreasing *n*
- are higher for ITO than for ZIO and In_2O_3:H

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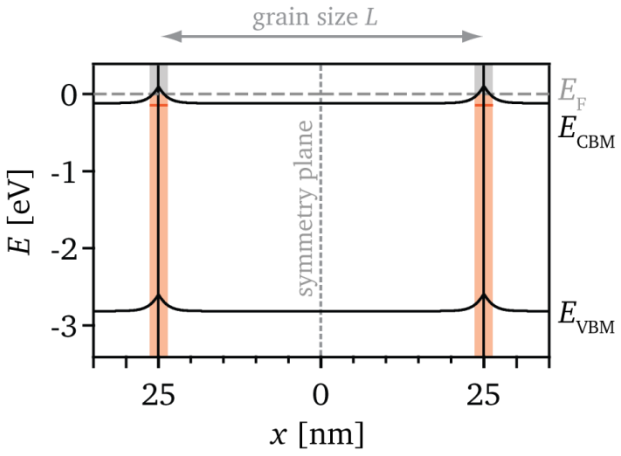
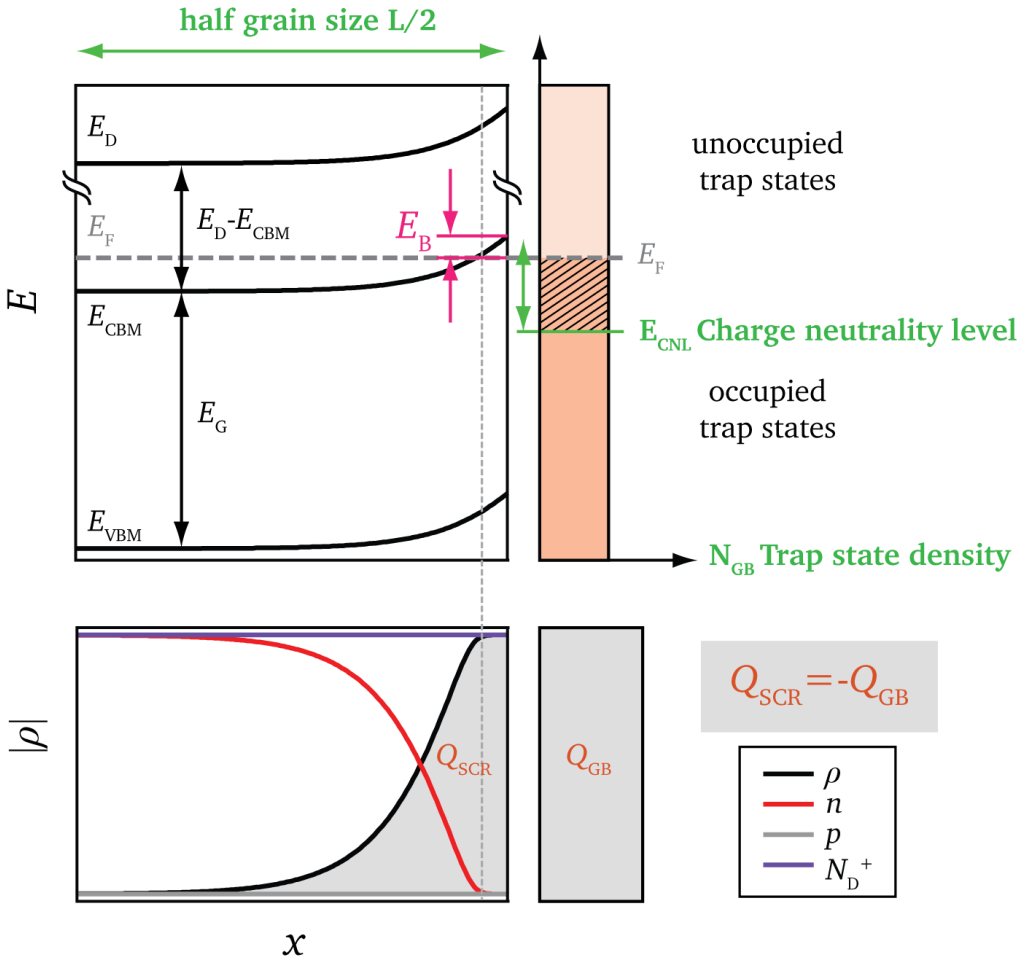
GB Scattering – Simulation: model





Literature

- „Setos modell“ was used:
  Not valid for degenerate semiconductors

Novel model needed

- Solving Poissons equation numerically

$$\rho(x) = -\epsilon_0 \epsilon_s \frac{d^2\phi(x)}{dx^2} = \epsilon_0 \epsilon_s \frac{d\mathscr{E}(x)}{dx}$$

- MATLAB simulation
- Parameters E_{CNL}, N_{GB}, L

GB Scattering – Simulation: results

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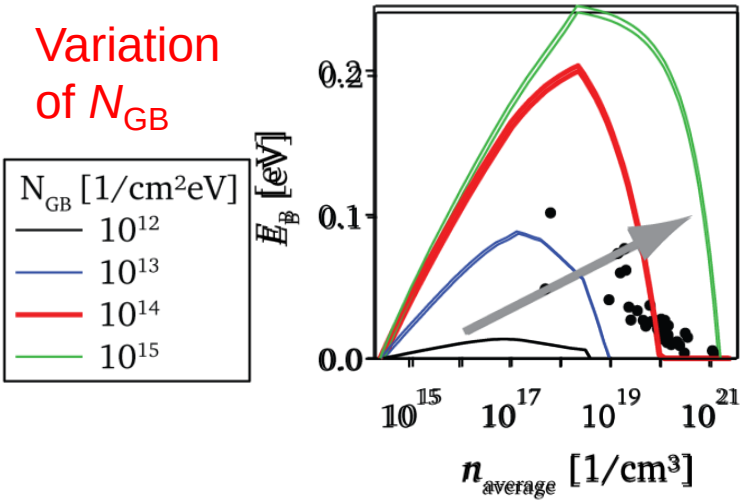
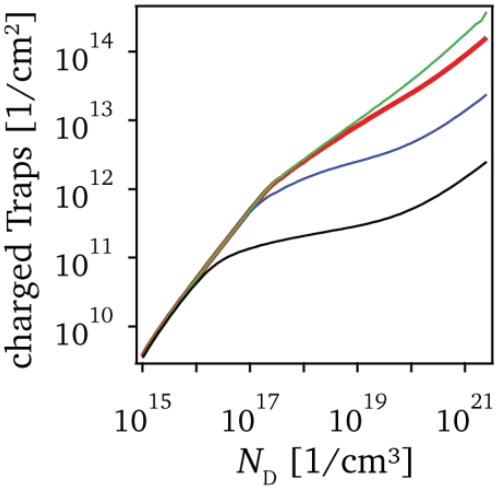
Variation of N_{GB}





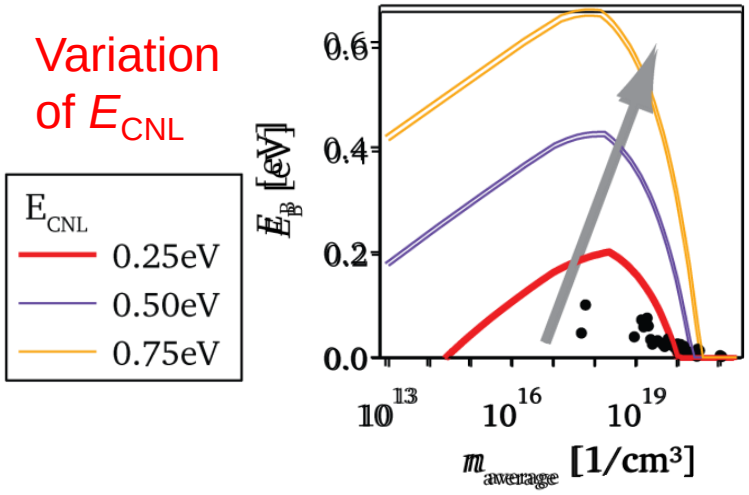
Standard Parameters

E_{CNL} = 0.25 eV

N_{GB} = 10^{14} /cm²eV

Grain size L = 50nm

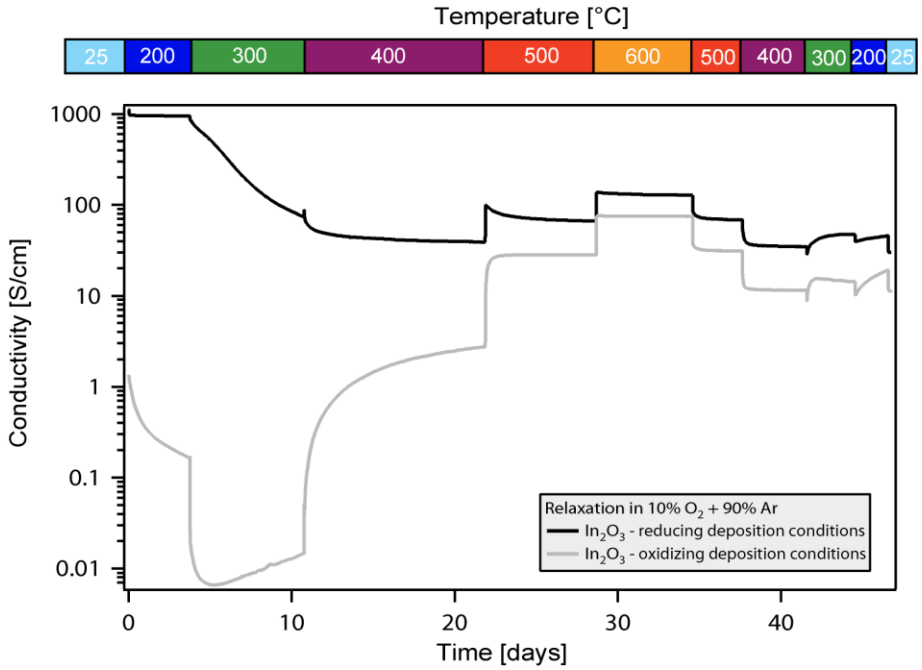
Variation of E_{CNL}



Model overdetermined for high n:
N_{GB} and E_{CNL} change position of onset

lower n necessary to measure maximum

THE experiment

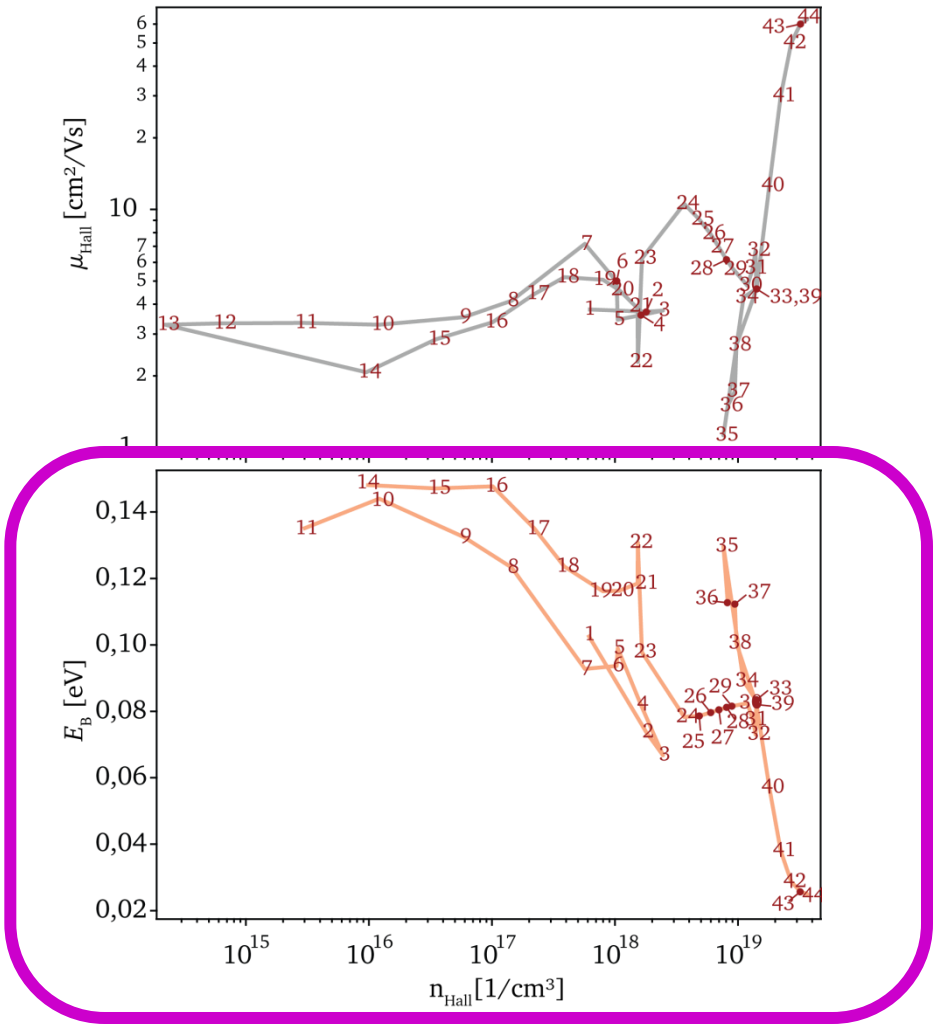


Sample:
Undoped In_2O_3 thin film deposited at oxidizing conditions

Relaxation measurement:
1. T-dependent
2. $p(O_2)$-dependent at 600°C

Cooling to RT after short time annealing and measurement of E_B

THE experiment - result



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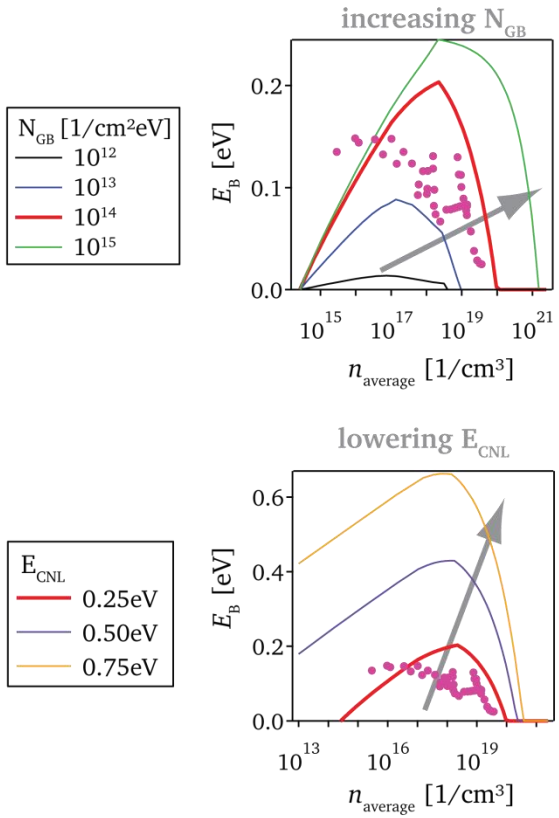
Relaxation measurement:
1. T-dependent
2. p(O_2)-dependent at 600°C

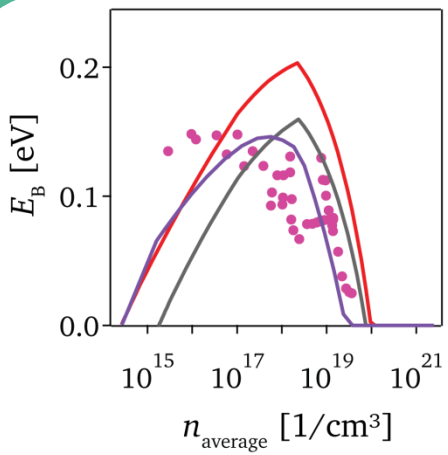
Cooling to RT after short time annealing and measurement of E_B

Total measurement time: 62 days

Comparison of measurement and simulation

Standard Parameters: E_{CNL}=0.25eV
N_{GB}=10^{14} 1/cm²eV
Grain size L= 50nm





E_{CNL}=0.25eV N_{GB}=10^{14} 1/cm²eV
E_{CNL}=0.25eV N_{GB}=**$3.2 \cdot 10^{13}$** 1/cm²eV
E_{CNL}=**0.20eV** N_{GB}=10^{14} 1/cm²eV

Approximate E_{CNL} and N_{GB} can be determined
E_{CNL}: 0.15eV to ~ max. 0.3eV
N_{GB}: 0.3-1 • 10^{14} 1/cm²eV

Summary

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- **Novel setup** for T and pO_2 dependent Hall-effect measurement was constructed
- In_2O_3 was doped with **Sn, Zr and H**: carrier concentration and mobility were analyzed
- **Grain boundary barriers E_B** were measured: doping element affects E_B
- Grain boundary scattering **model** was developed and and grain barrier hight simulated
  - **One In_2O_3 sample** was measured about large carrier concentration region: E_{CNL} and N_{GB} can be simulated (first time!)

Thank you very much for your attention!