ISOLDE Workshop and Users meeting 2013

Origin of unusual Ag diffusion profiles in CdTe

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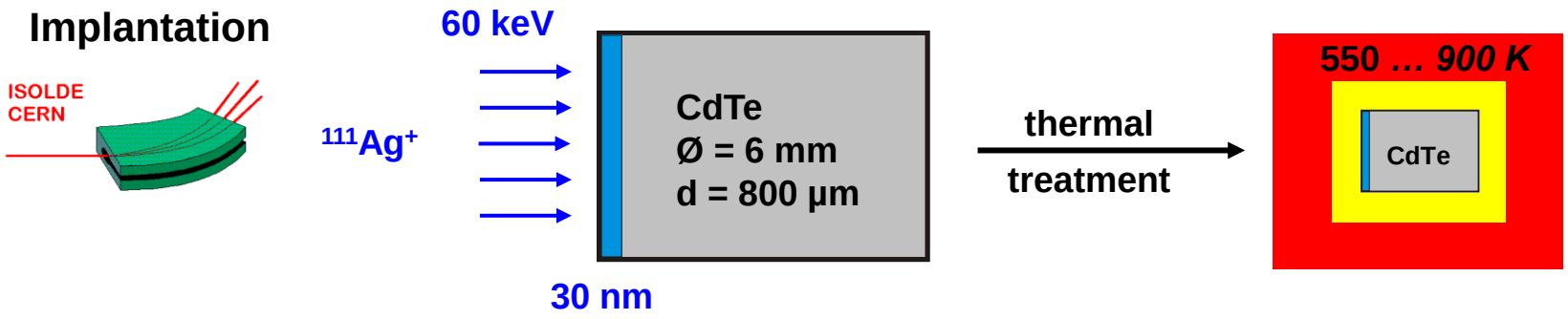
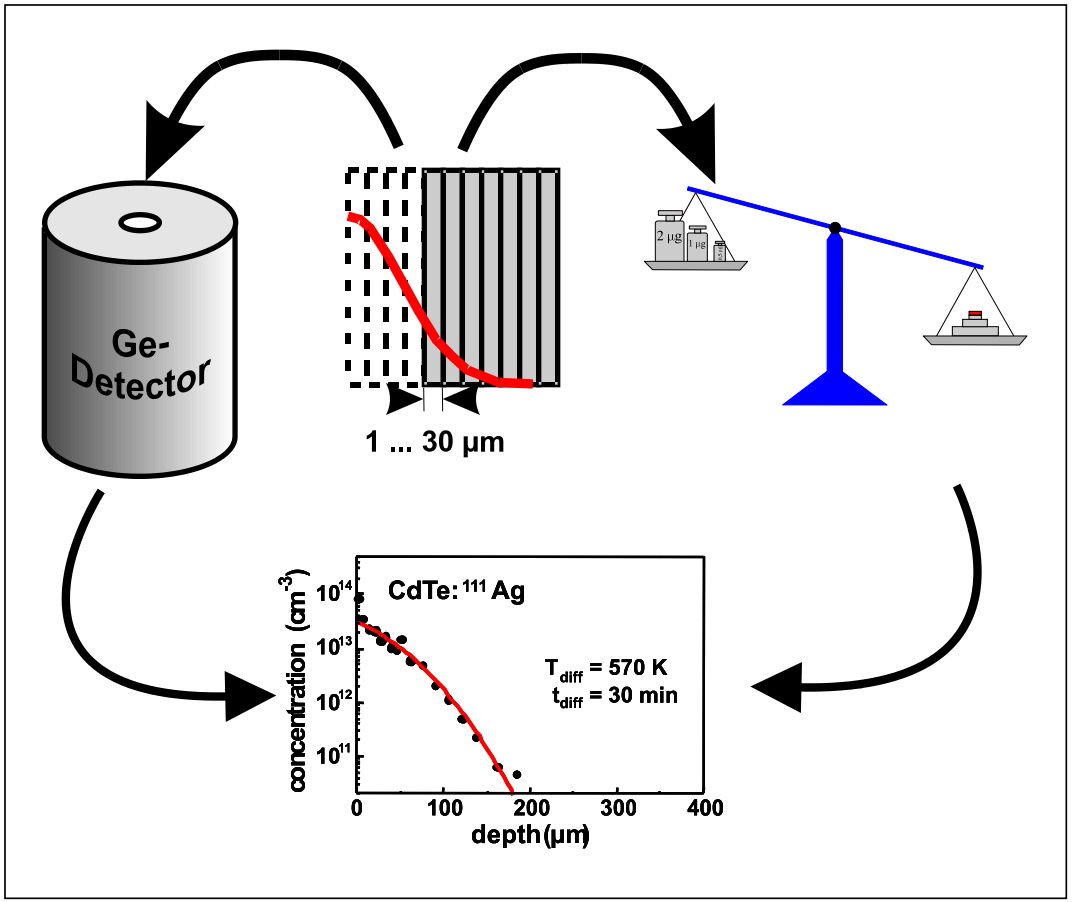
Outline

- **Diffusion**
- **Uphill diffusion of Ag in CdTe**
- **Influence of metal layers on Ag diffusion**
- **Influence of oxidized crystal surfaces**
- **Summary**

Radiotracer technique





Mechanical sectioning

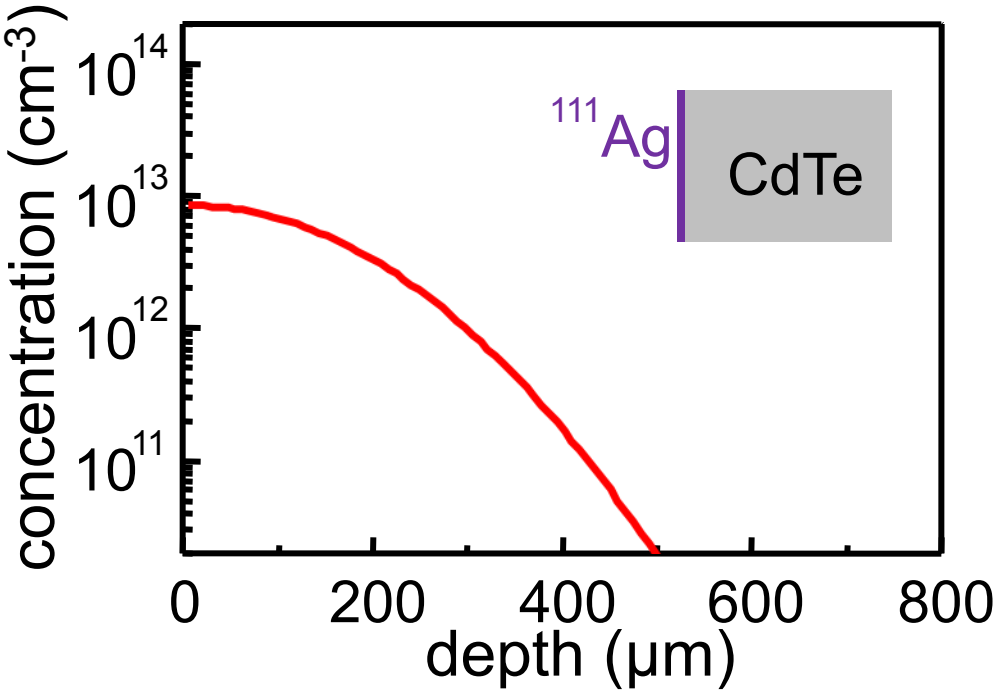
- Resolution > 1 µm
- $T_{1/2}$ > 1 h

3

Diffusion in solids

$$J(X) = -D_X \frac{\partial [X]}{\partial x}$$

$$\frac{\partial [X]}{\partial t} = -\frac{\partial}{\partial x} J(X)$$

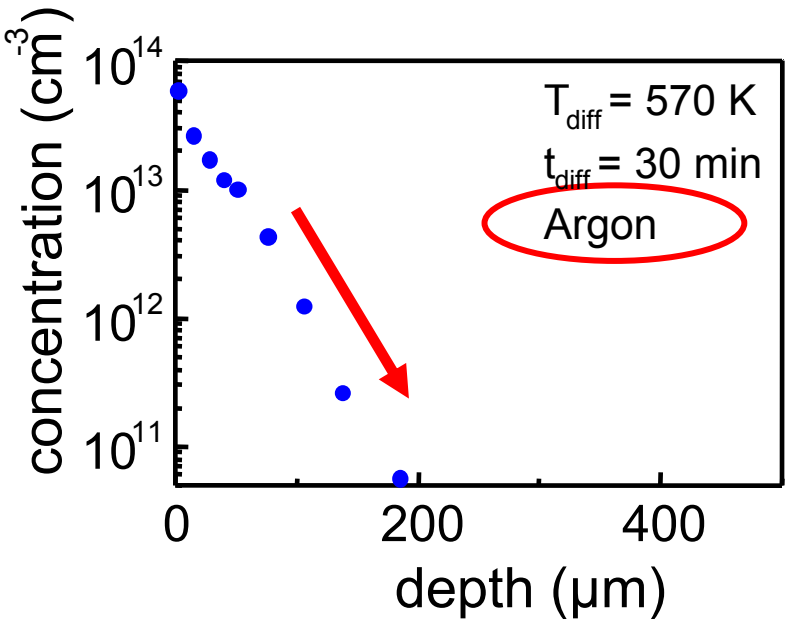


for $C(x, t=0) = N \cdot \delta(x)$

$$C(x,t) = \frac{N}{\sqrt{2\pi \cdot Dt}} \cdot e^{-\frac{x^2}{4Dt}}$$

Monotonously decreasing profiles

Diffusion of ^{111}Ag in CdTe



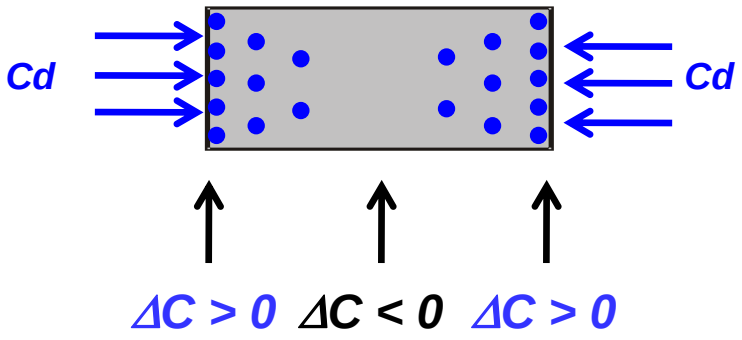
Monotonously decreasing profile

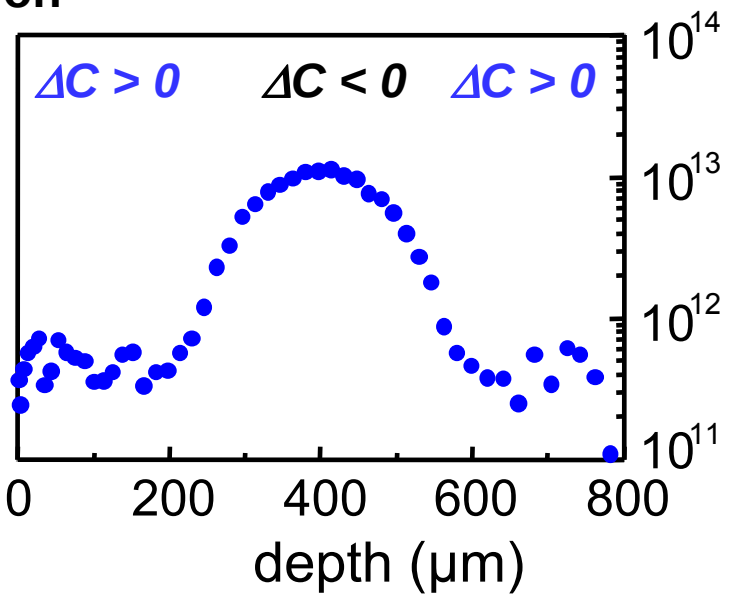
Uphill diffusion profile

(H. Wolf *et al.*, Phys. Rev. Lett. 94 (2005) 125901)

Model

- **Deviation from stoichiometry** $[\Delta C]=[Cd_i]-[V_{Cd}]$
- **Initial state of the crystal Te rich** $\Delta C < 0$
- **Highly mobile Cd interstitials**
- **Highly mobile Ag dopant (interstitial)**
- **Source of Cd interstitials during diffusion**





- **Ag dopants images the profile of the intrinsic defects**

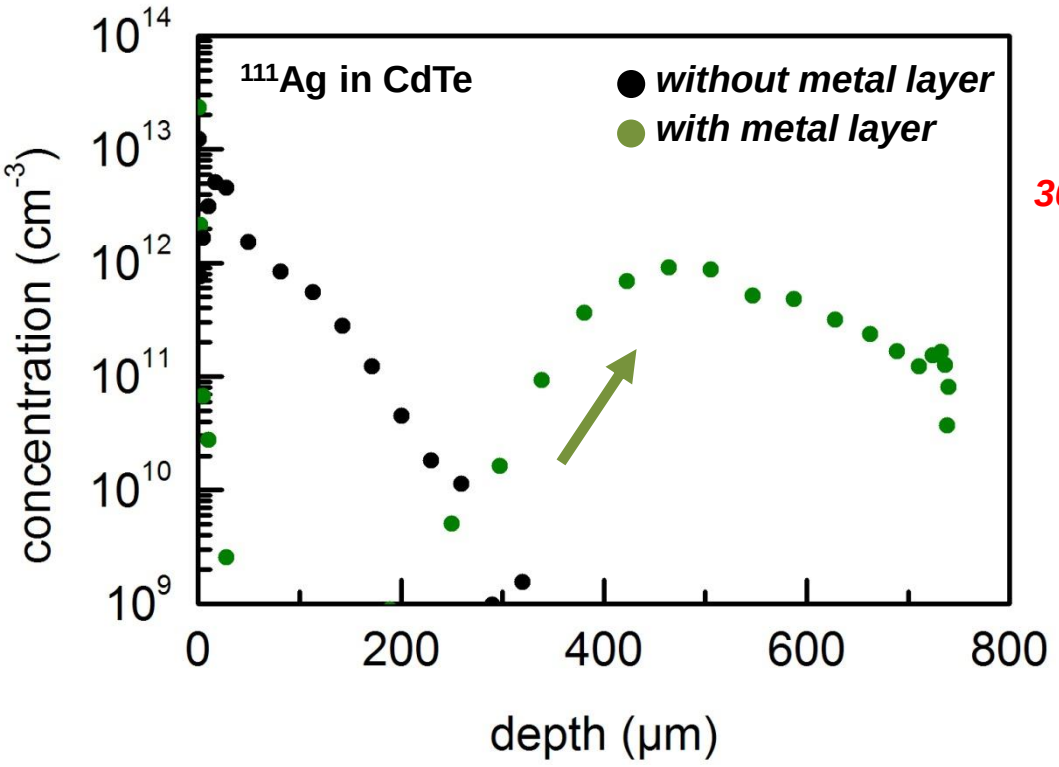
Alternative sources for Cd_i defects?

- **Metal layers**

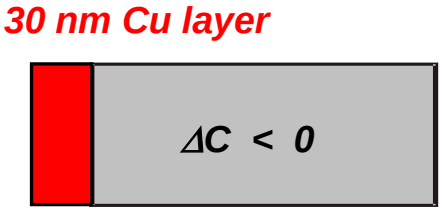
- **Oxidized crystal surfaces**

Influence of metal layers (Cu)

Diffusion without Cu layer at 500 K



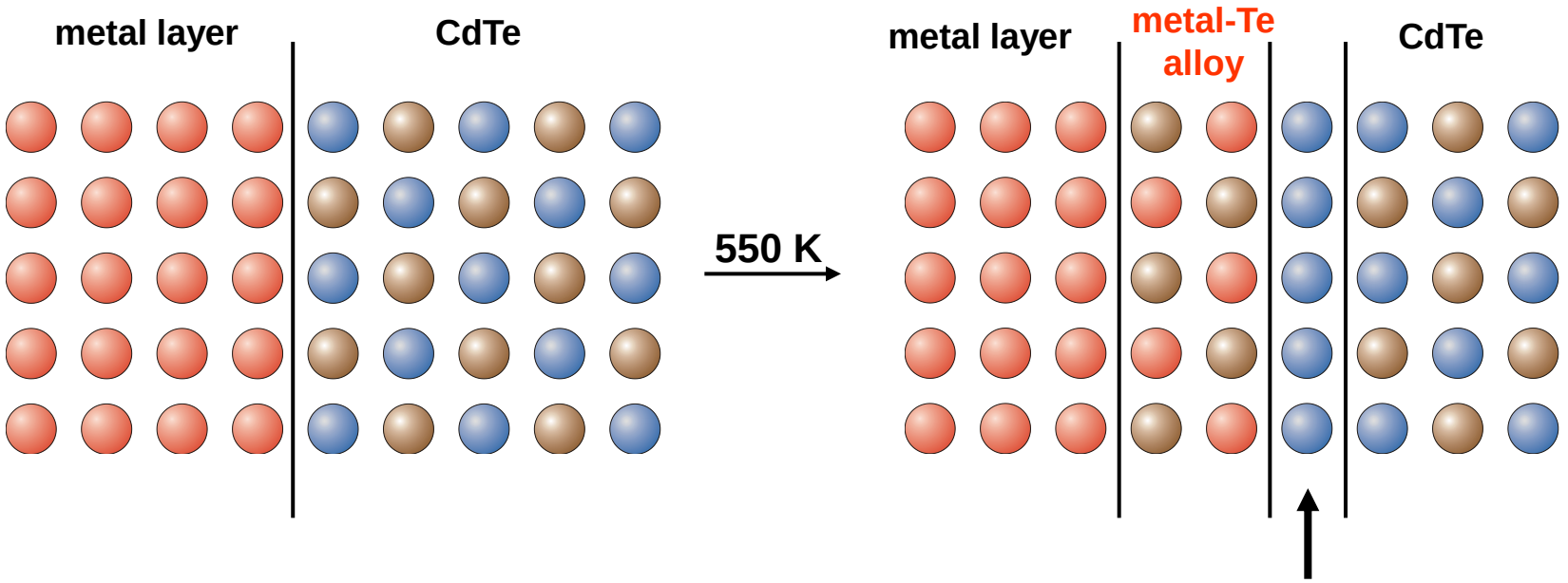
Cu layer at 500 K

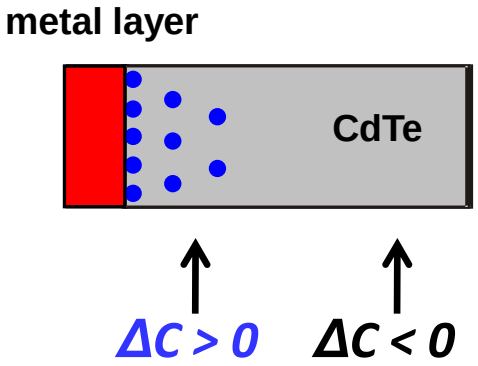


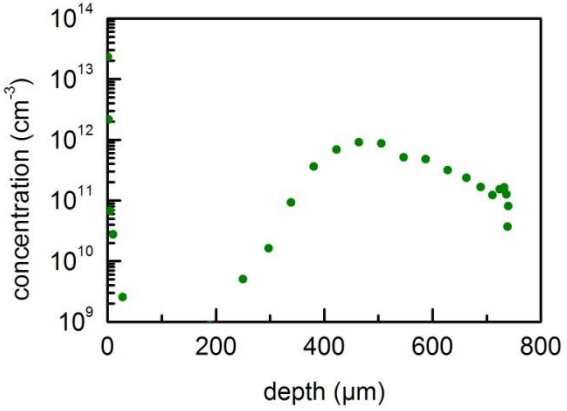
Metal layers can initialize uphill diffusion

(H. Wolf *et al.*, Appl. Phys. Lett. 100 (2012) 171915)

Model

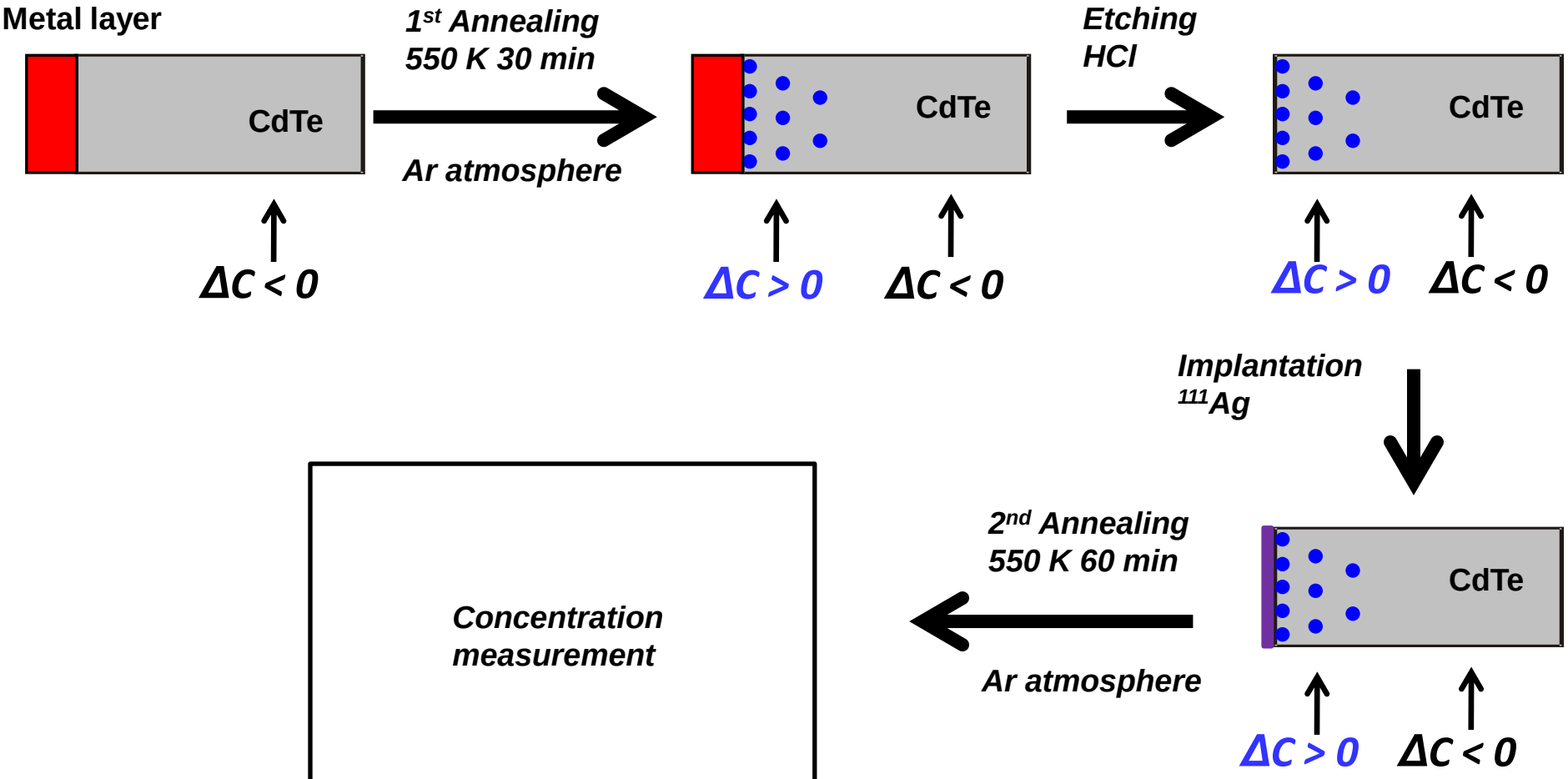






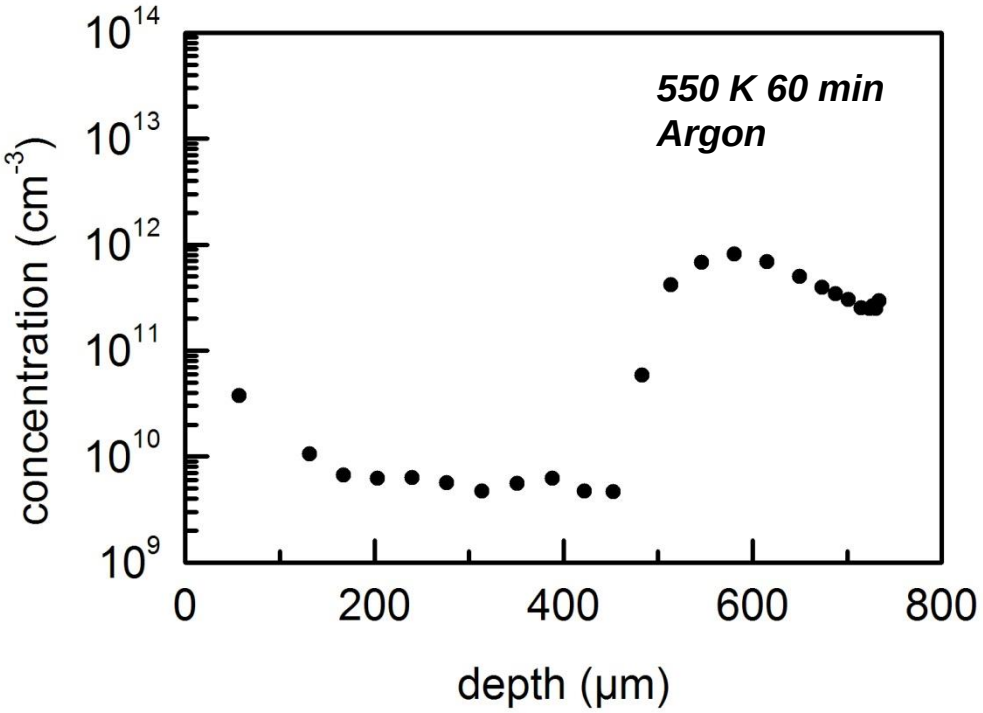
Ag dopant images the profile of deviation of stoichiometry again?

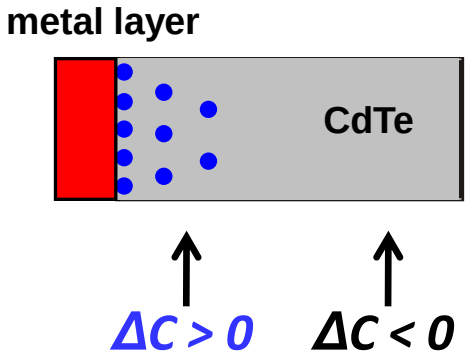
Can Ag image a previously prepared deviation of stoichiometry?



Creating the deviation of stoichiometry before implantation of Ag

Experimental result

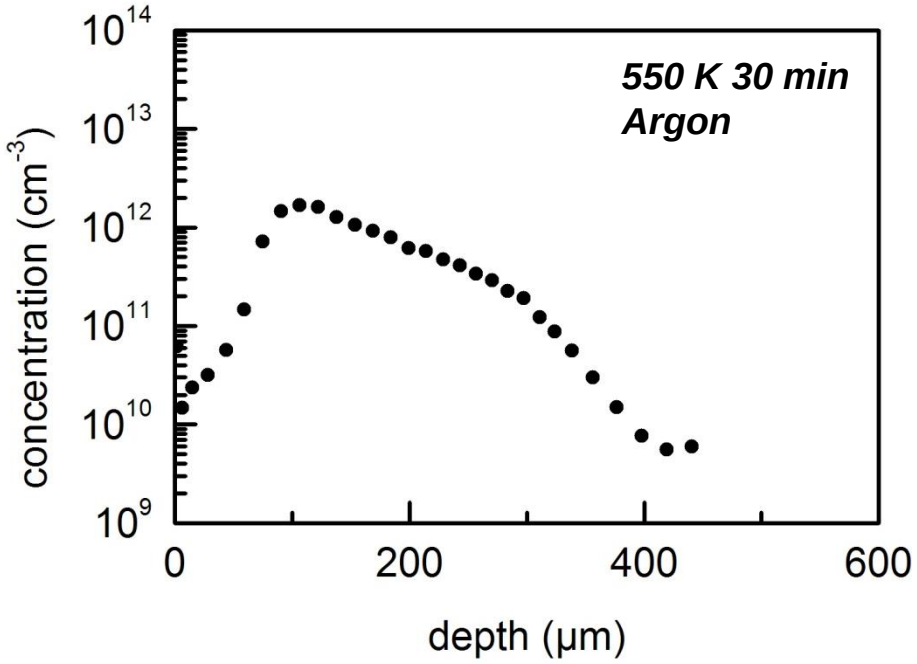




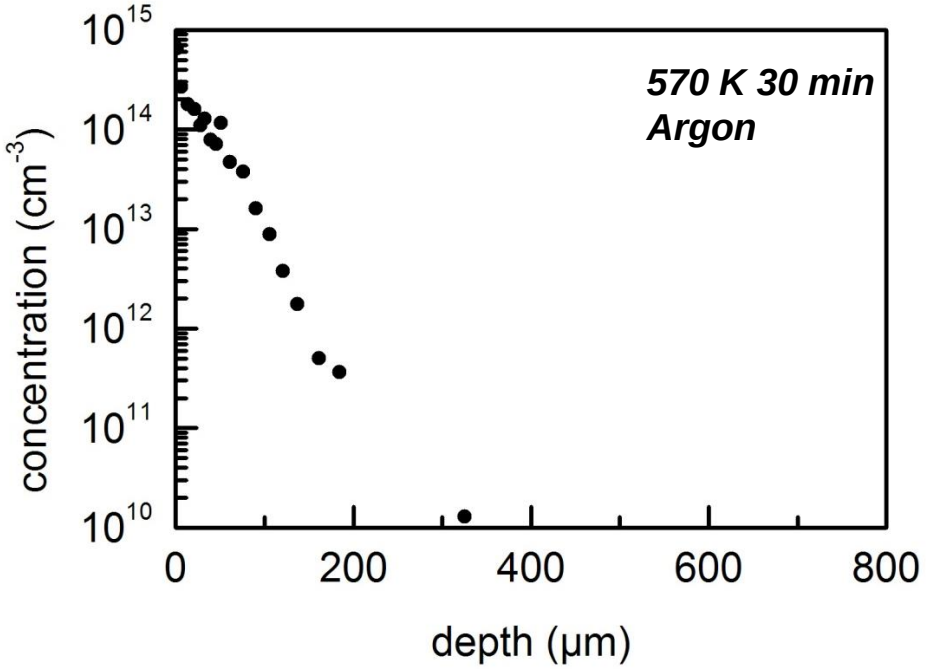
- Cd source is created by Te-metal alloy
- Concentration of the dopant images the profile of deviation from stoichiometry again
- Can we create a Cd source at the surface without evaporated metals?

Influence of the condition of the crystal surface

as delivered



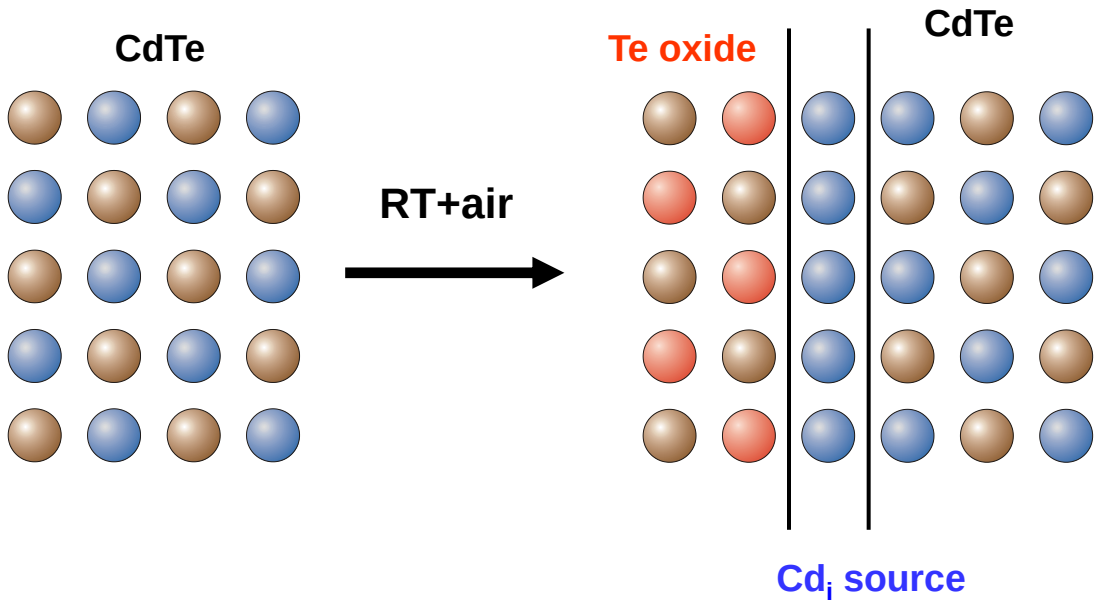
etched (Br-methanol, KOH)



- As delivered samples show uphill diffusion
- Br-methanol, KOH etching suppresses uphill diffusion
- Surface condition has significant effect on Ag diffusion

Mechanism

- Natural oxidation at room temperature and air [1)]
- TEM measurements: TeO_2 at the surface [2)]
- No evidence of Cd at the surface



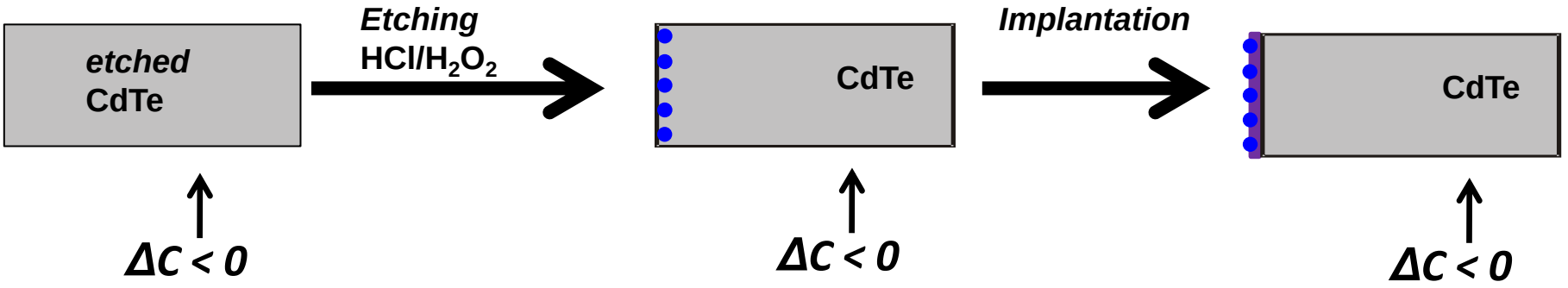
- Cd source is created by natural oxidation process

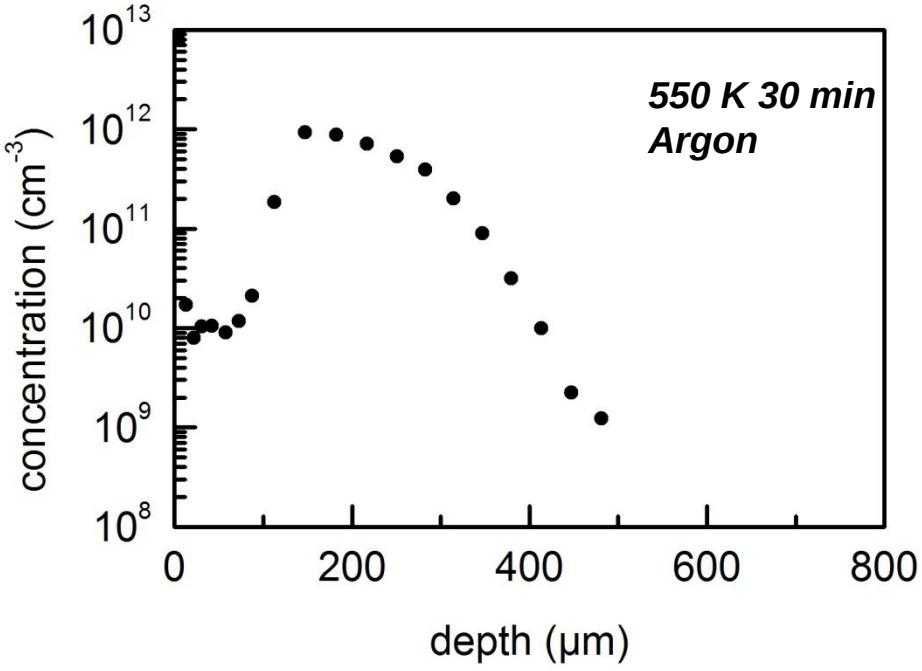
- Can we create a Cd source by oxidizing etching?

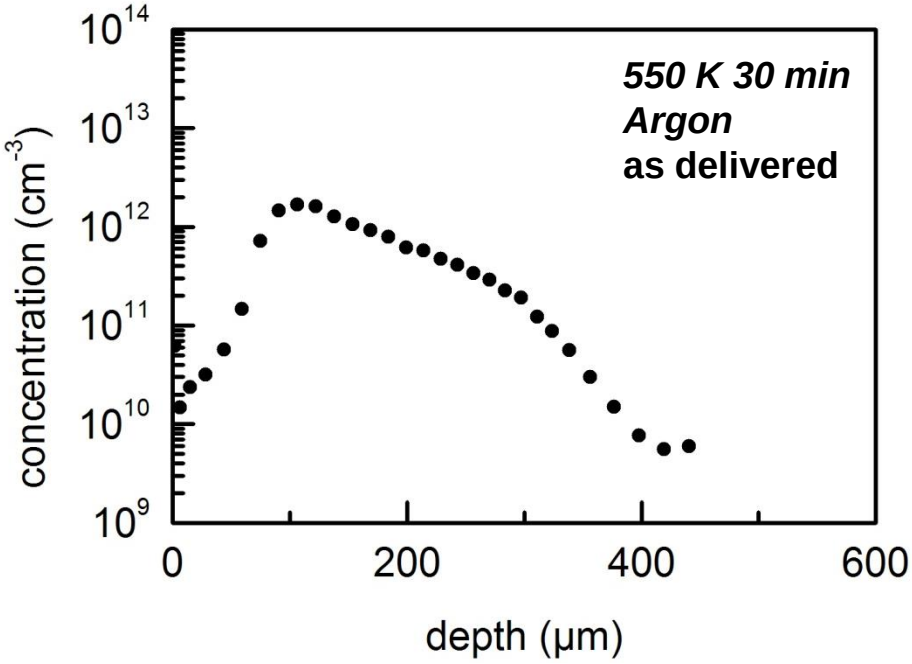
1) *T. B. Wu, J. S. Chen, C. D. Chiang, Y. M. Pang, and S. J. Yang, J. Appl. Phys. 71, 5212 (1992)*

2) *F. A. Ponce, R. Sinclair, and R. H. Bube, Appl. Phys. Lett. 39, 951 (1981)*

Experimental idea





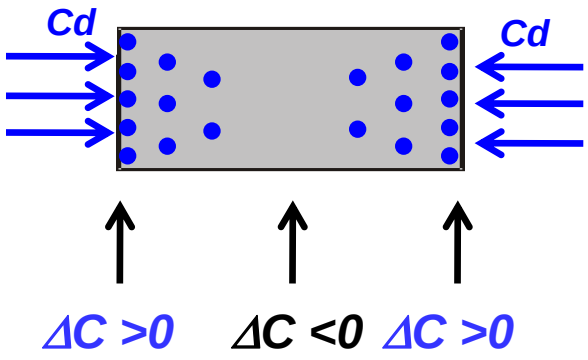


- **Oxidation creates a Cd source**

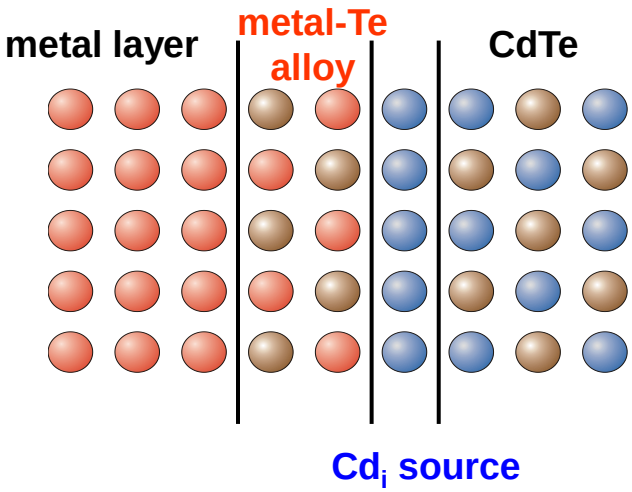
Summary

- Uphill diffusion is initialized by a Cd source
- Ag dopant images the profile of the deviation from stoichiometry
- Cd source can be provided by:

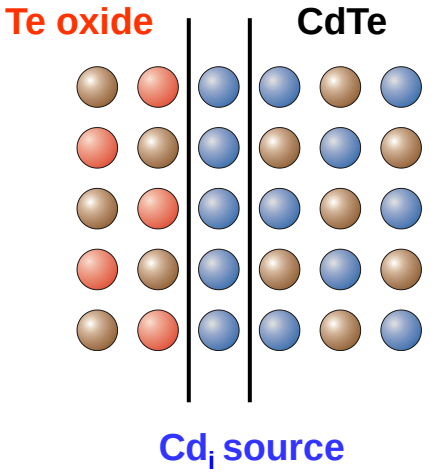
external Cd pressure



evaporated metal layer



natural and forced oxidation



Outlook

➢ Verifying of the results by diffusion experiments AND observation of the state of the surface (XPS or similar method)

Thanks to

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CERN:

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