First observation of new diffusion phenomena in CdTe

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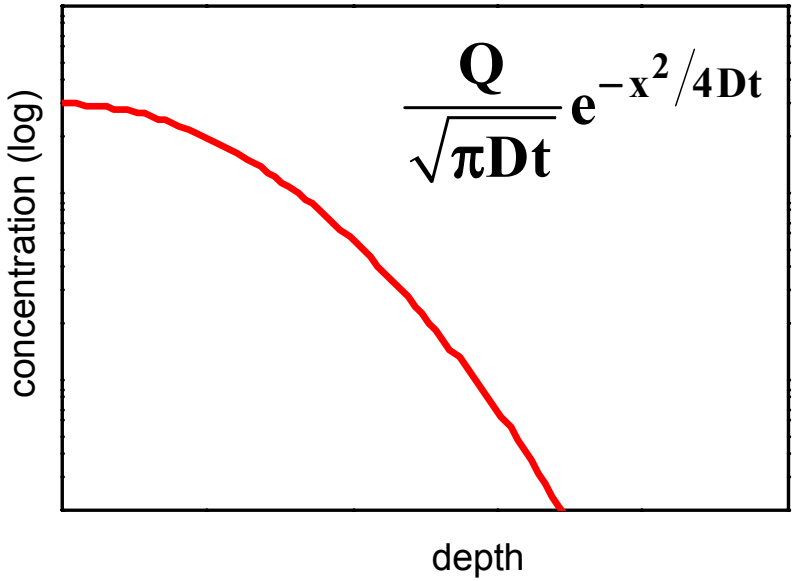
Diffusion in solids

Fick's first law: $$j(Ag) = -D_{Ag}\frac{\partial[Ag]}{\partial x}$$

Fick's second law: $$\frac{\partial[Ag]}{\partial t} = -\frac{\partial}{\partial x} j(Ag)$$

Solution for finite source



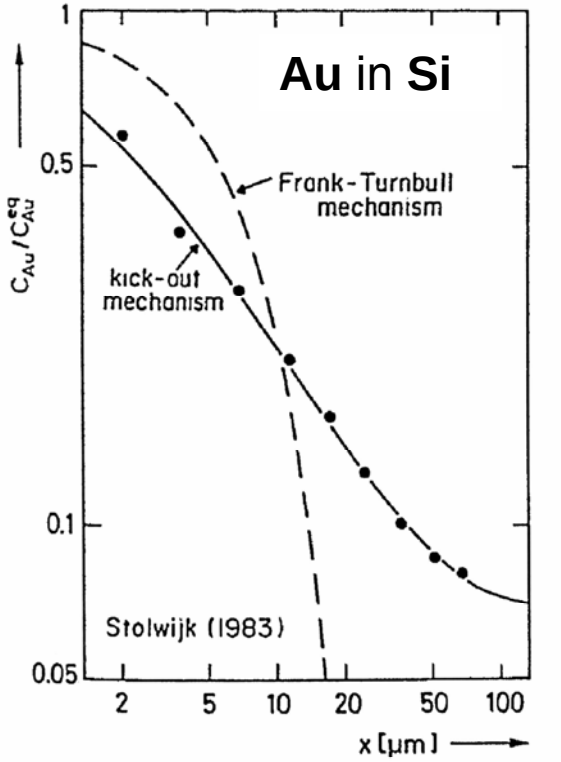
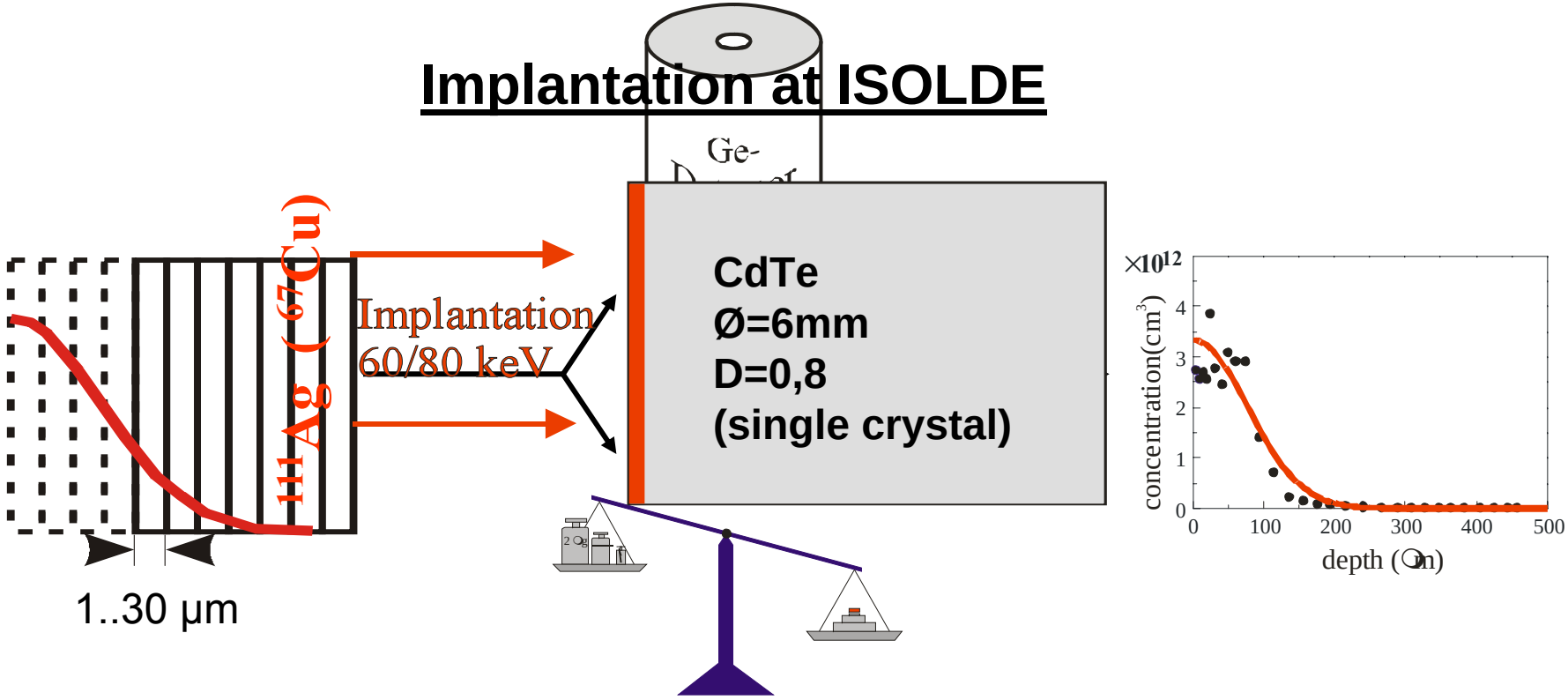


Figure 5-10. Experimental gold concentration profile in dislocation-free silicon (solid circles) compared with predictions of the Frank-Turnbull and the kick-out mechanism (Stolwijk et al., 1983).

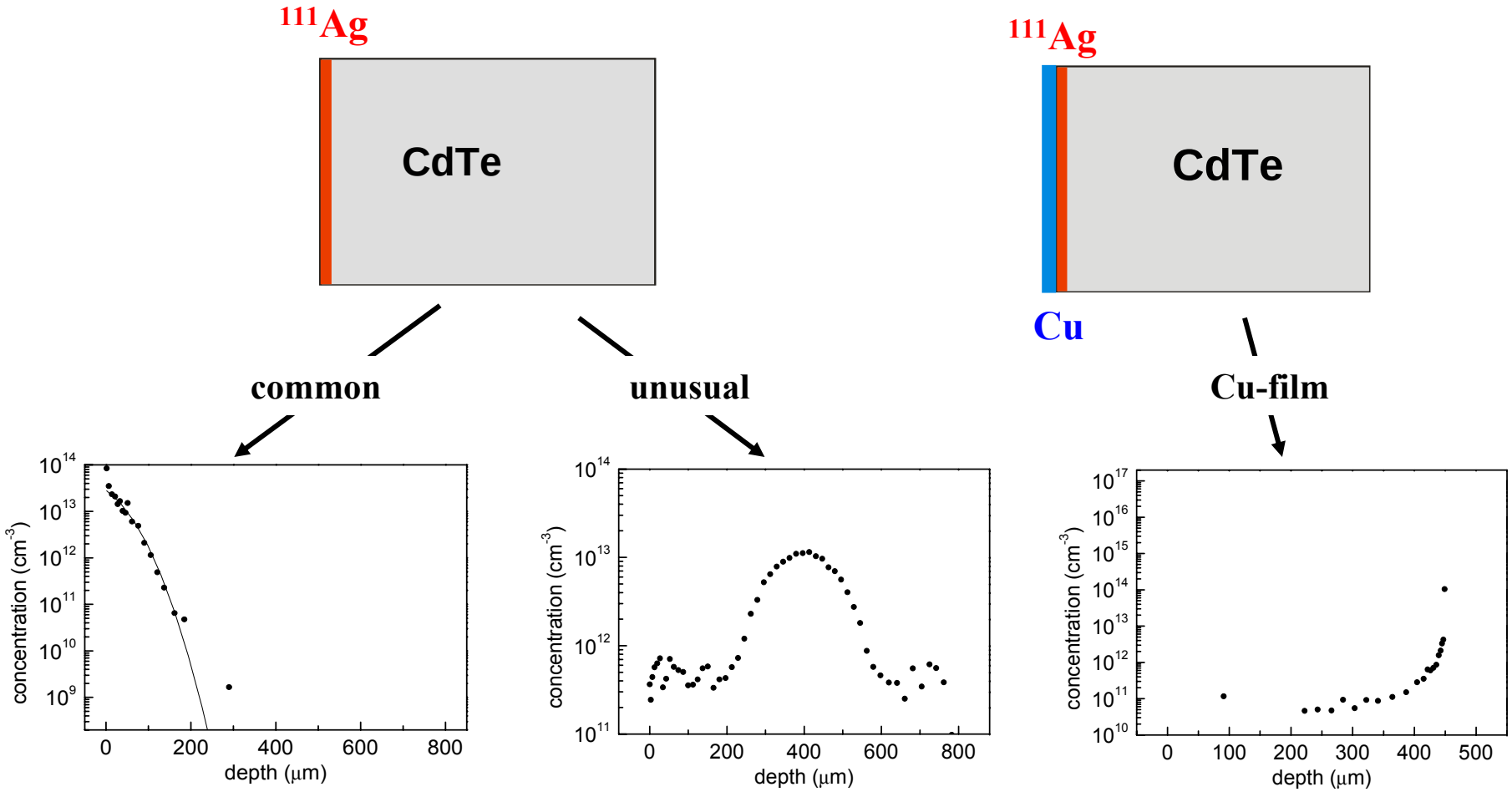
N.A. Stolwijk, B. Schuster, J. Hölzl, H. Mehrer and W. Frank, Physica 116 B,. 335 – 342, (1983)

Monotonously decreasing profiles

Experimental details



Motivation

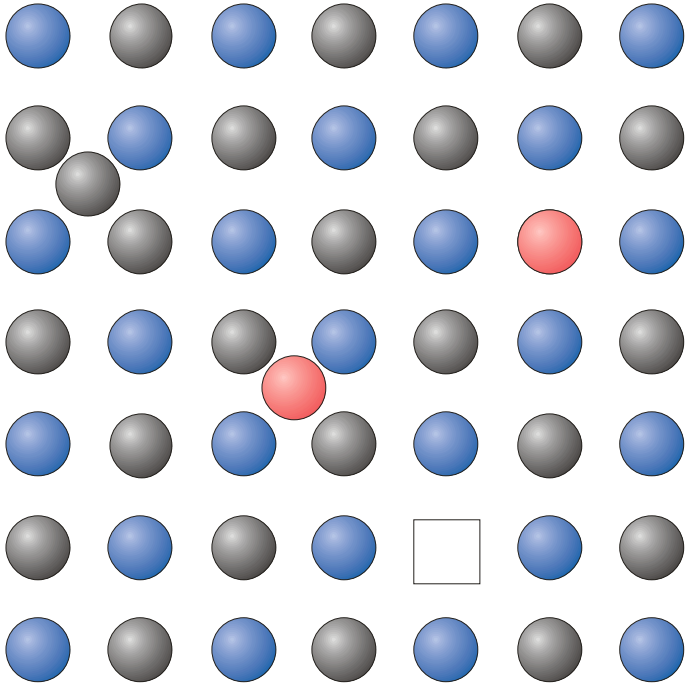


*) Wolf, H., Wagner, F., Wichert, Th., and ISOLDE Collaboration, *Phys. Rev. Lett.* 94, 2005 , 125901

Unexpected, new profile forms *)

Diffusion of Ag under Cd-atmosphere

Defects in CdTe



Extrinsic defects

Ag: Ag_{Cd}, Ag_i

Intrinsic defects

Cd: Cd_i, V_{Cd}

Te sub lattice: perfect

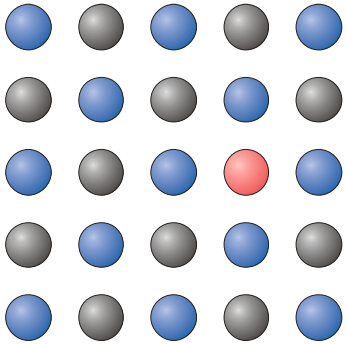
$[Cd_i]$-$[V_{Cd}]$: *deviation from stoichiometry*

reflected by: $\frac{[Cd_i]}{[V_{Cd}]}$

Defect reaction and thermal equilibrium

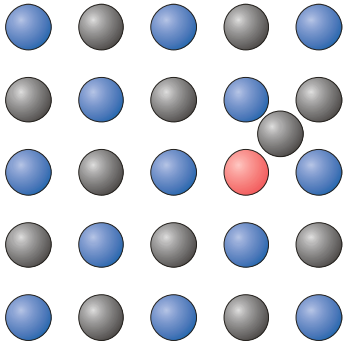
Ag in CdTe

dissociative



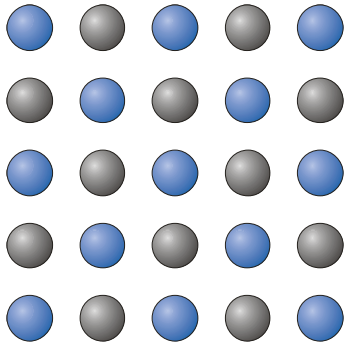
$$Ag_i + V_{Cd} \leftrightarrow Ag_{Cd}$$

kick-out

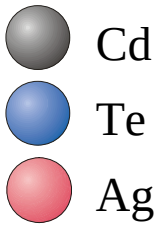


$$Ag_i \leftrightarrow Ag_{Cd} + Cd_i$$

annihilation



$$Cd_i + V_{Cd} \leftrightarrow 0$$

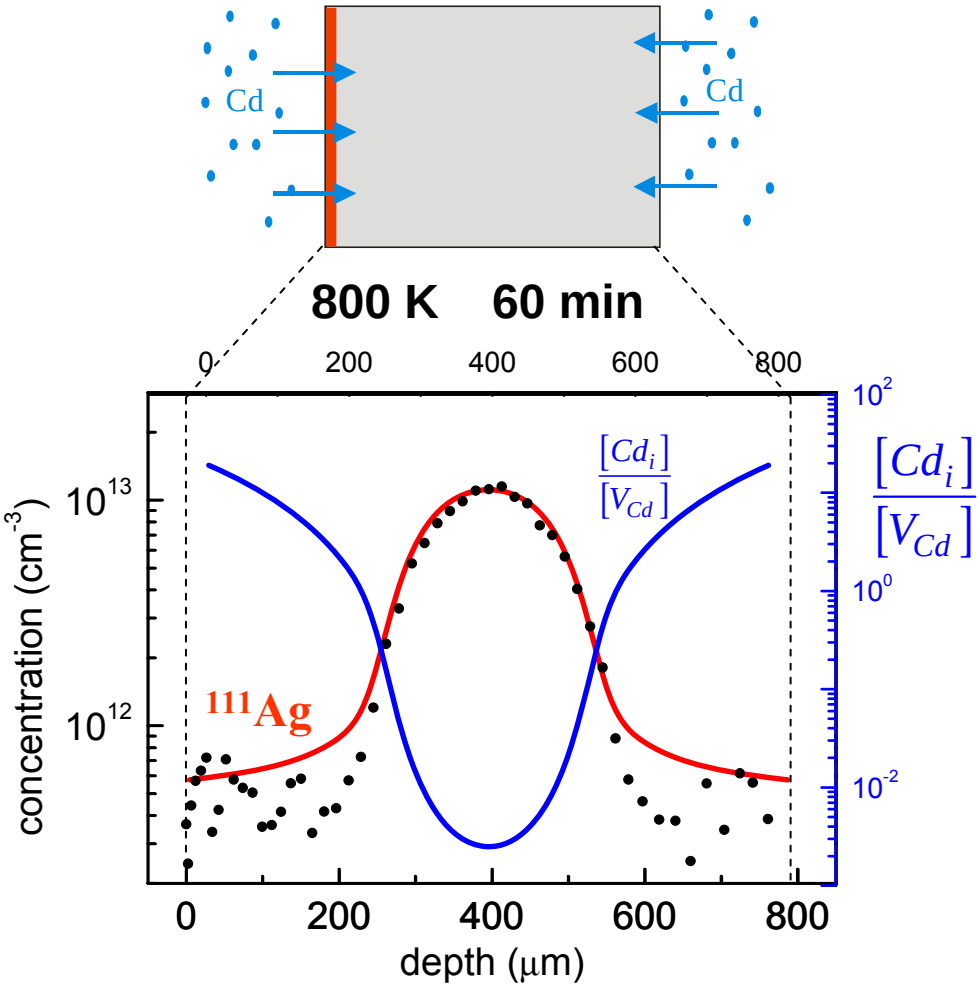


local equilibrium

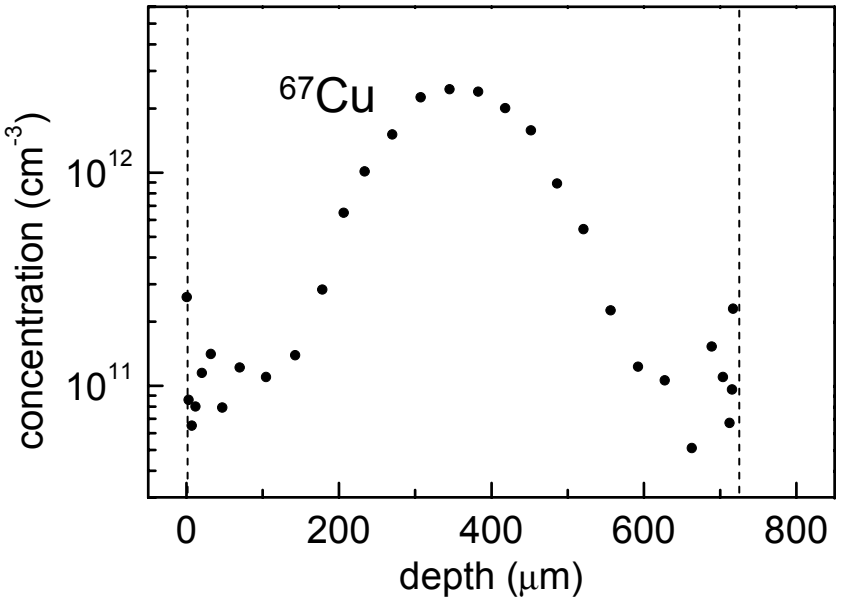
$$\frac{[Ag_i]}{[Ag_{Cd}]} = K\sqrt{\frac{[Cd_i]}{[V_{Cd}]}}$$

Changes in the stoichiometry

Ag in CdTe: Cd-atmosphere



- high mobility of Ag_i (Cu_i)
- low mobility of Ag_{Cd} (Cu_{Cd})

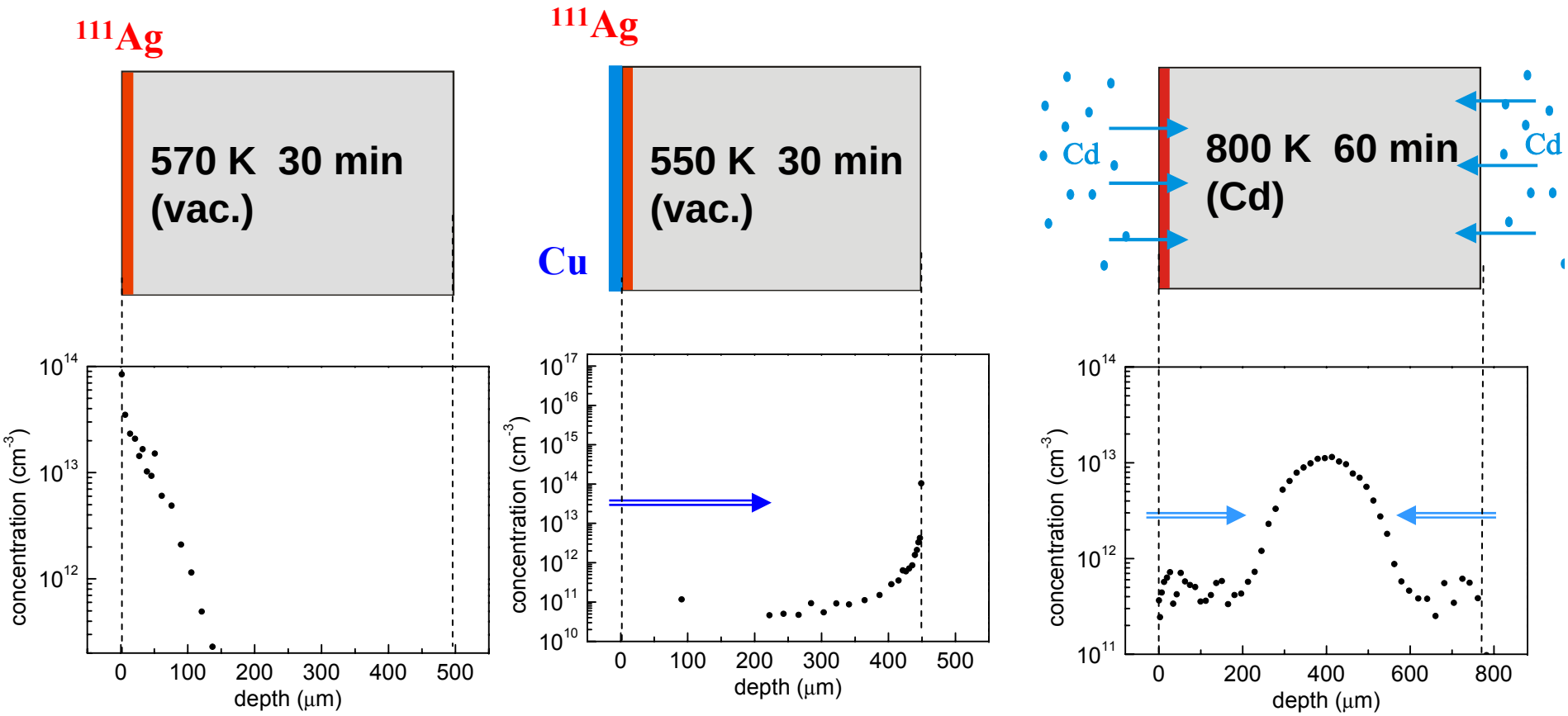


Ag-profile reflects the stoichiometry of the crystal

- Unusual diffusion profiles observed in CdTe
- Strong influence of the deviation from stoichiometry
- Model based on defect reactions

Codiffusion of Ag and Cu

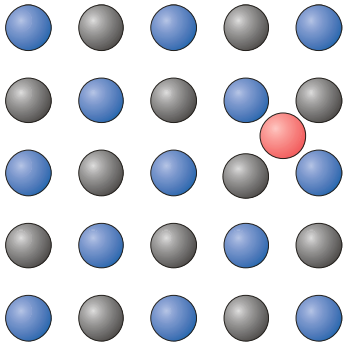
Codiffusion of Ag with Cu in CdTe



Similarities between codiffusion of Cu and diffusion under Cd-atmosphere

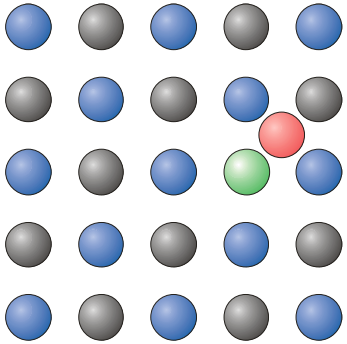
Codiffusion: Important defect reactions

kick out



$$Cd_i + Ag_{Cd} \leftrightarrow Cd_{Cd} + Ag_i$$

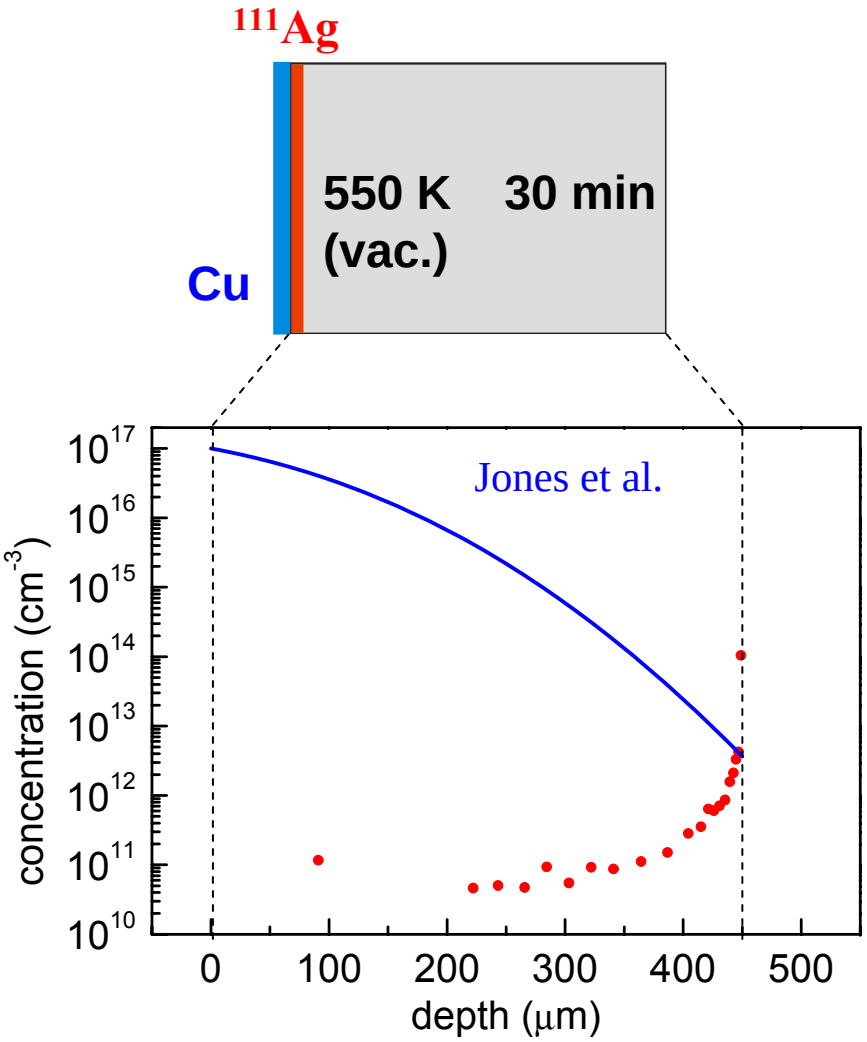
codiffusion



$$Cu_i + Ag_{Cd} \leftrightarrow Cu_{Cd} + Ag_i$$

Analogous behavior of Cd_i and Cu_i

Codiffusion of Ag und Cu

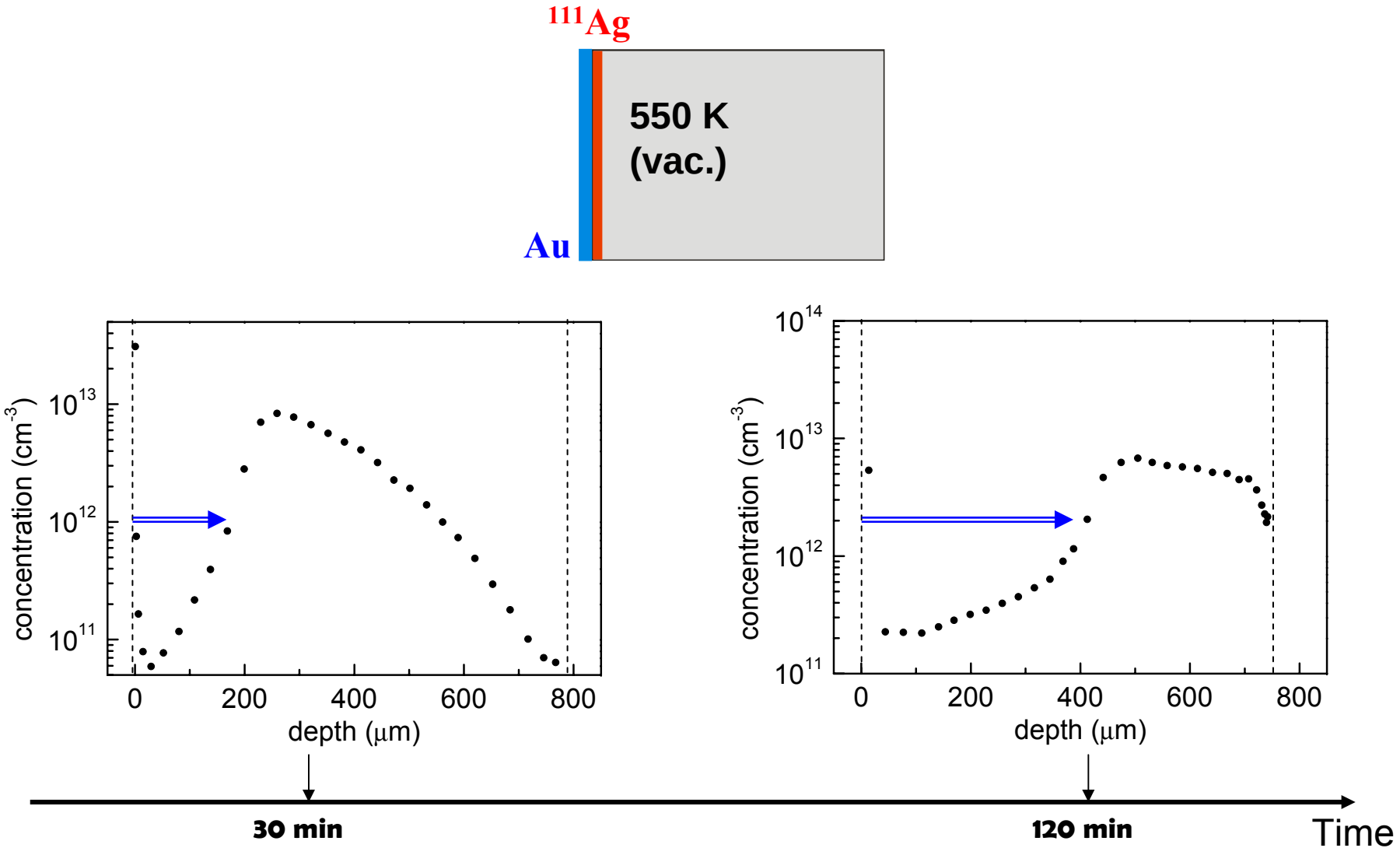


E.D.Jones, N. M. Stewart, J. B. Mullin, J.Crystal Growth 117, 244 (1992)

Ag-profile reflects the Cu distribution

Codiffusion of Ag and Au

Codiffusion Ag and Au



Similar effect to Cu-codiffusion

Summary

Ag diffusion under Cd atmosphere

- uncommon profile forms
- distribution of Ag reflects the sample stoichiometry

Codiffusion of Ag and Cu or Au

- replacement of Ag by Cu and Au

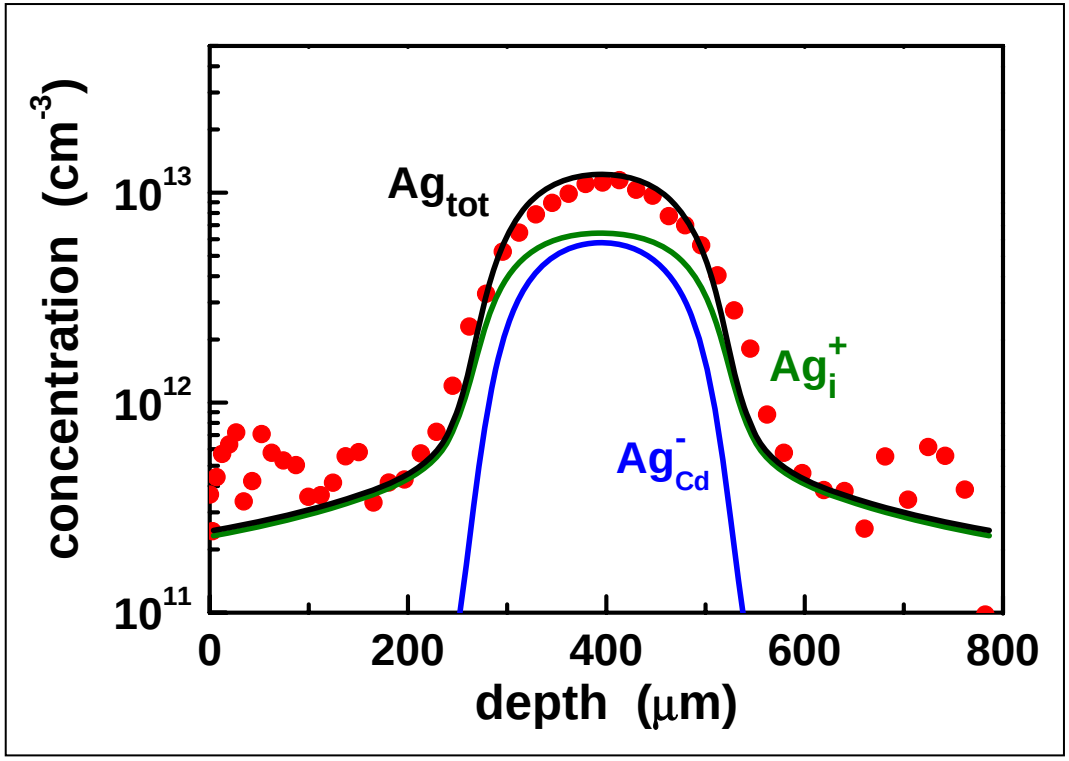
Modell based on defect reaction

$$Cd_i + Ag_{Cd} \leftrightarrow Cd_{Cd} + Ag_i$$
$$Cu_i + Ag_{Cd} \leftrightarrow Cu_{Cd} + Ag_i$$
$$Au_i + Ag_{Cd} \leftrightarrow Au_{Cd} + Ag_i$$

State of the art

Charged defects:

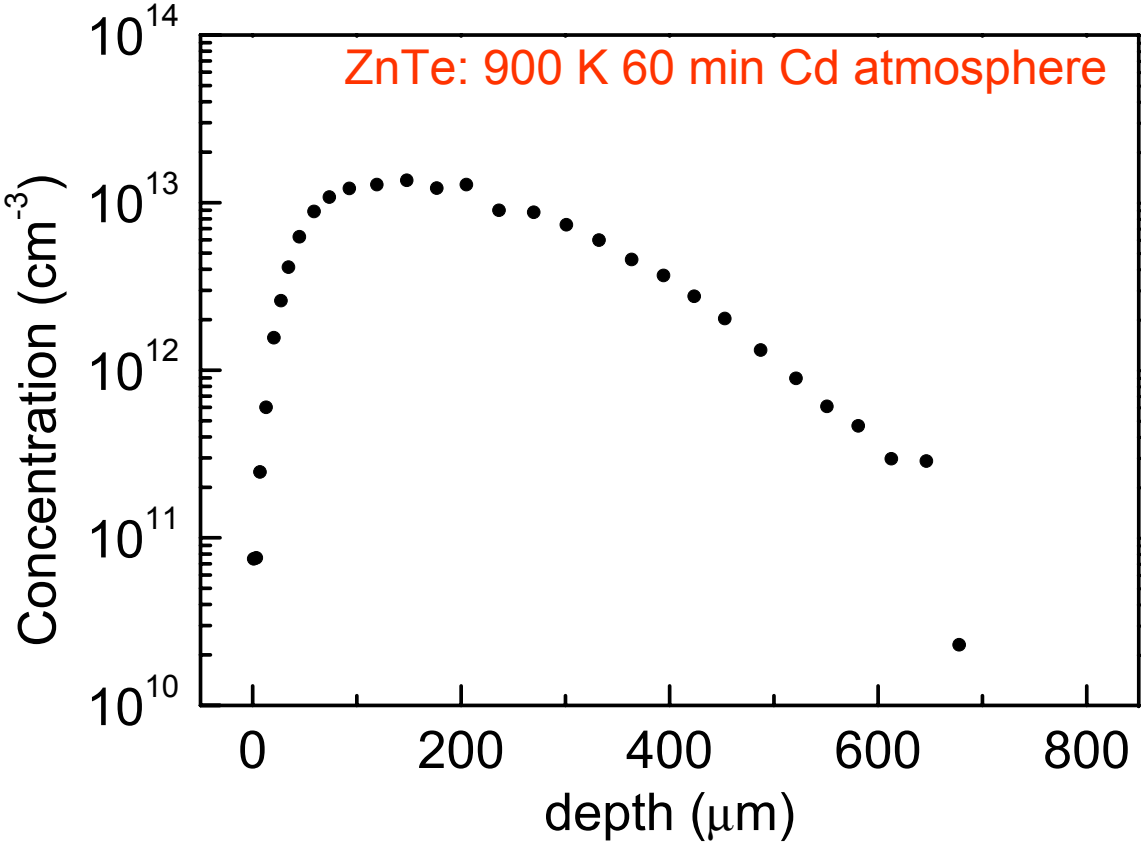
- donor: Ag_i^+ Cd_i^+
- acceptor: Ag_{Cd}^- V_{Cd}^-



Outlook: Matrix

Matrix:

- CdTe
- **II-VI** Semiconductors
- **III-V** semi conductors



Outlook: diffusing element

Diffusing element:

- ^{111}Ag; ^{67}Cu
- acceptor
- donor
- magnetic dopant