Diffusion of charged native defects in semiconductors: The case of CdTe

Roman Grill
E.Belas, J.Franc, P.Höschl, P.Moravec

Institute of Physics, Charles University,
Ke Karlovu 5, CZ-121 16 Prague 2, Czech Republic
e-mail: grill@karlov.mff.cuni.cz

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Objectives

- Theoretical explanation of the formation of detector-grade CdTe
- Optimization of growth process to fit predicted demands

Detector-grade CdTe

1. High resistivity

$\rho = 10^9 - 10^{10}\ \Omega cm$ $E_F \approx E_g/2;\ E_g \approx 1.5$ eV at 300 K

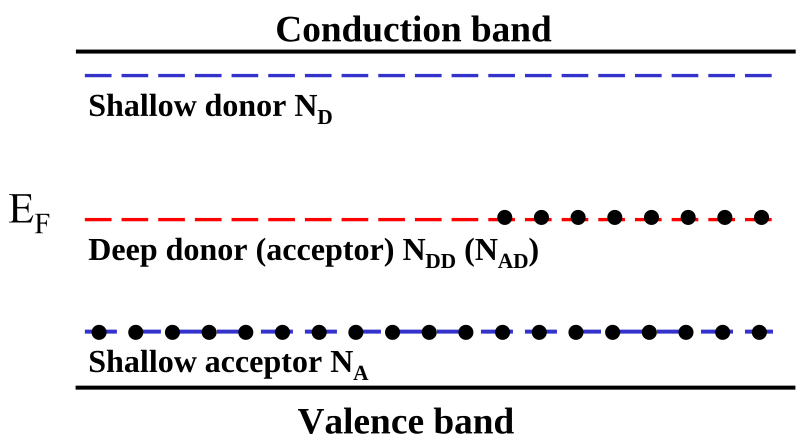
$n;\ p = 10^6 - 10^7\ cm^{-3}$ $n_i(300K) = 8\times10^5\ cm^{-3}$

A. Shallow donors and acceptors $N_D \approx N_A > 10^{15}\ cm^{-3}$

$|\,N_D - N_A\,| = 10^6 - 10^7\ cm^{-3}$ nonrealizable

B. Shallow donors and acceptors + deep donor/acceptor

(N_{DD}/N_{AD}) $N_{DD} + N_D > N_A > N_D$ / $N_{AD} + N_A > N_D > N_A$



at uncorrelated donor-acceptor doping

$\Rightarrow N_{DD}(N_{AD}) > 10^{15}\ cm^{-3}$

Detector-grade CdTe

2. Large life-time; low trap density

$$\tau = \frac{1}{\upsilon_T \sigma N_t}$$

thermal velocity
(steady at respective T)

capture cross-section $\sigma \approx 10^{-15}$ cm^2
(reduction of killers with σ up to 10^{-11}cm^2)

trap density

Demand in detector-grade CdTe: **$N_t < 10^{13}$ cm^{-3}**

$N_{DD}(N_{AD}) > 10^{15}$ cm^{-3}
$N_t < 10^{13}$ cm^{-3}

⇒Search for a model of high resistivity with a low midgap level density

Defect modelling – quasi-chemical formalism

List of included point defects

Native defects:

- Cd interstitial (Cd_I), divalent donor, dominates in Cd-rich CdTe
- Cd vacancy (V_{Cd}), divalent acceptor, dominates in Te-rich CdTe
- Te antisite (Te_{Cd}), multivalent donor, dominates in Te-rich CdTe, missing experimental evidence

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Shallow extrinsic donor (e.g. In_{Cd}, Cl_{Te})

Native defect related complex: ($V_{Cd}D$) ≡A-center, acceptor

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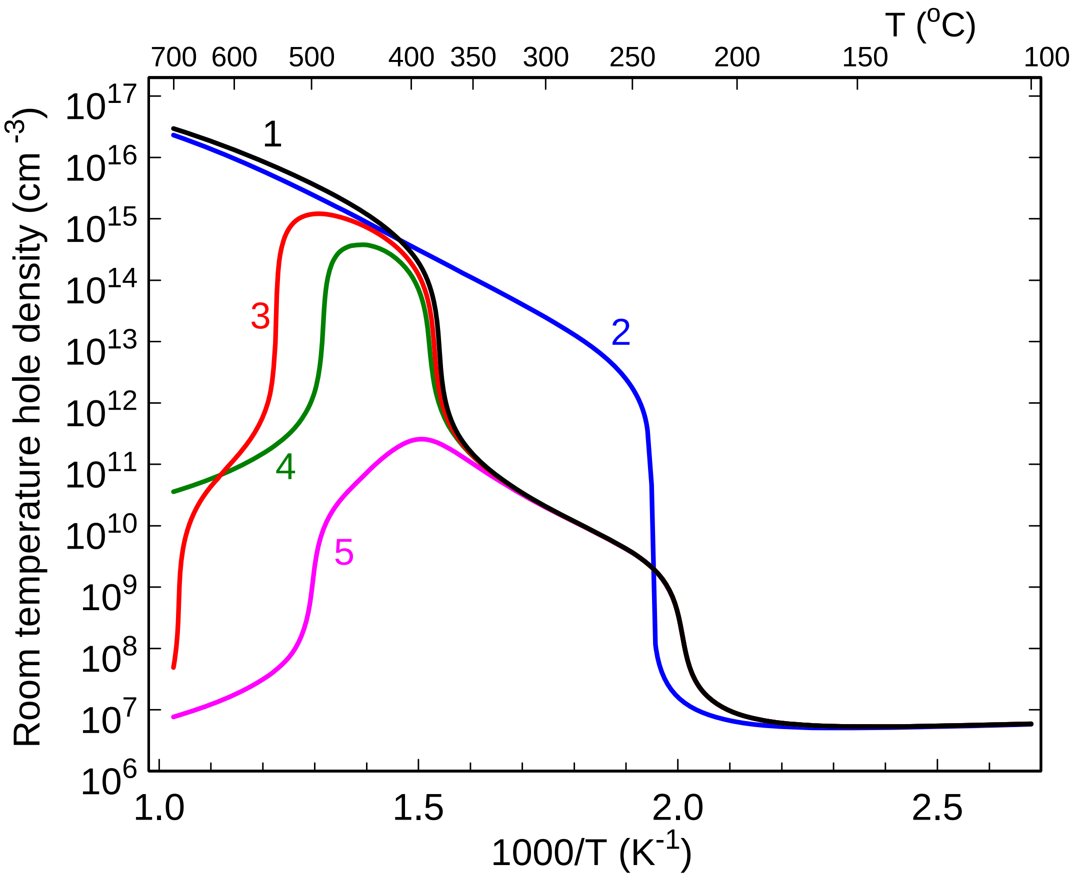
Midgap level with a low density 10^{13} cm^{-3}

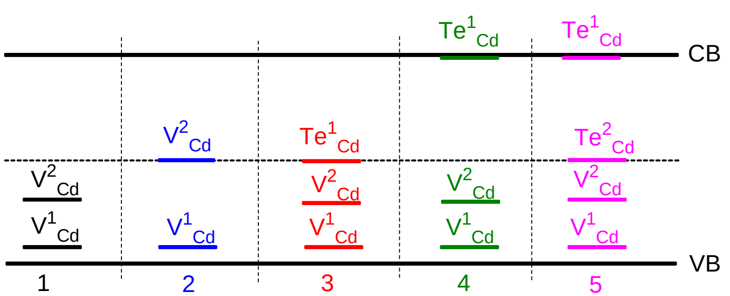
Native defect properties are consistent with high-temperature transport and thermodynamic data.

Extremely high self-compensation of shallow donors by Cd vacancies and A-centers at defect equilibrium at low temperature T<250^{0}C.



Te-saturated CdTe with shallow donor 10^{15}cm^{-3}, midgap level 10^{13}cm^{-3}, and A-centre included.

Five defect models



R.Grill et al., IEEE Trans. Nucl. Sci. 52, 1925 (2005).

Question

How to achieve Te-saturated defect equilibrium at low T?

Detailed study of point defect diffusion and relaxation is necessary.

Chemical diffusion - theory

Chemical flux of q-charged defect X

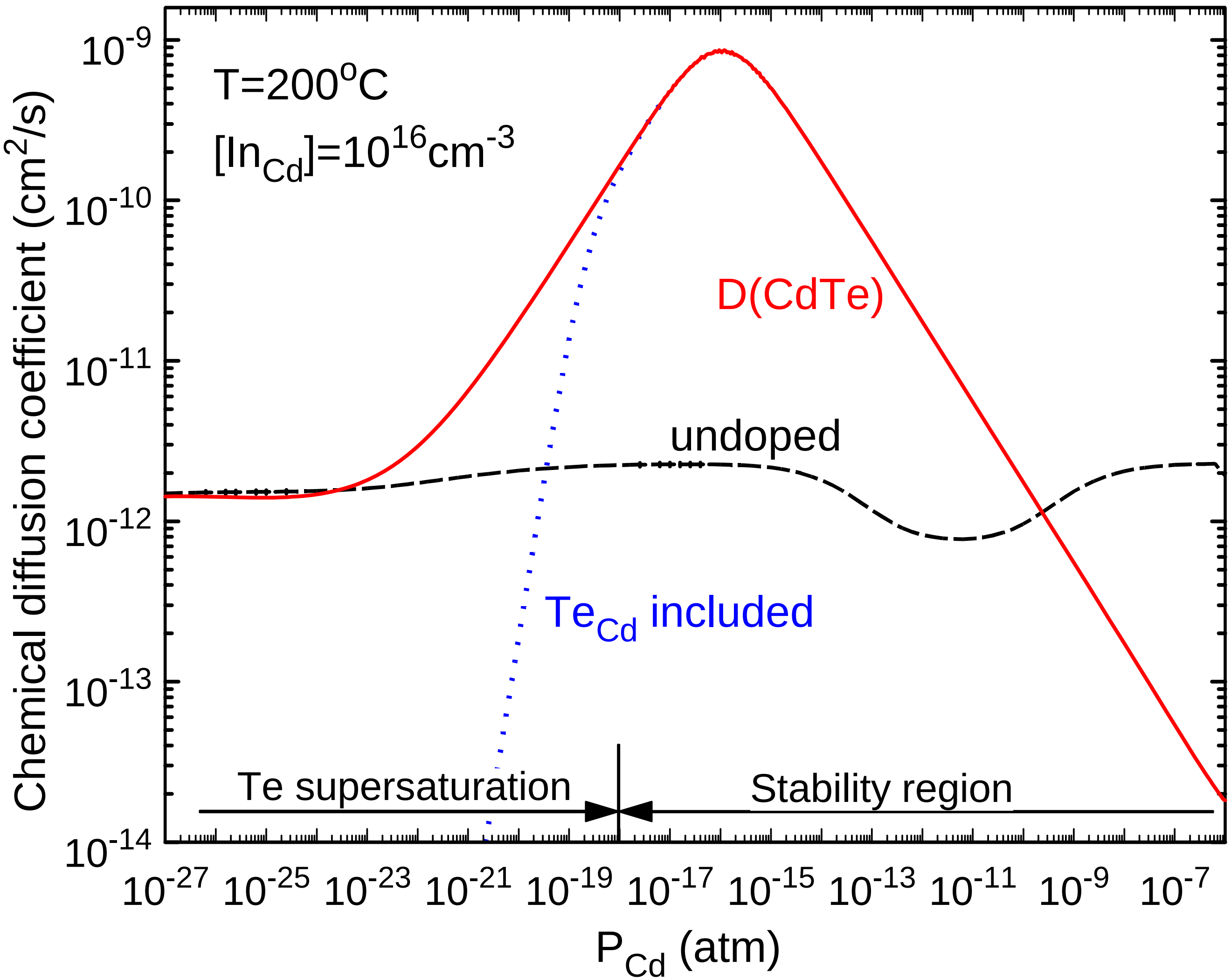
$$J_X^q = -D_X^q \frac{d[X^q]}{dz} + < v_X^q > [X^q] = -D_X^q \frac{X^q}{X^0} \frac{d[X^0]}{dz}$$

Coefficient of chemical self-diffusion

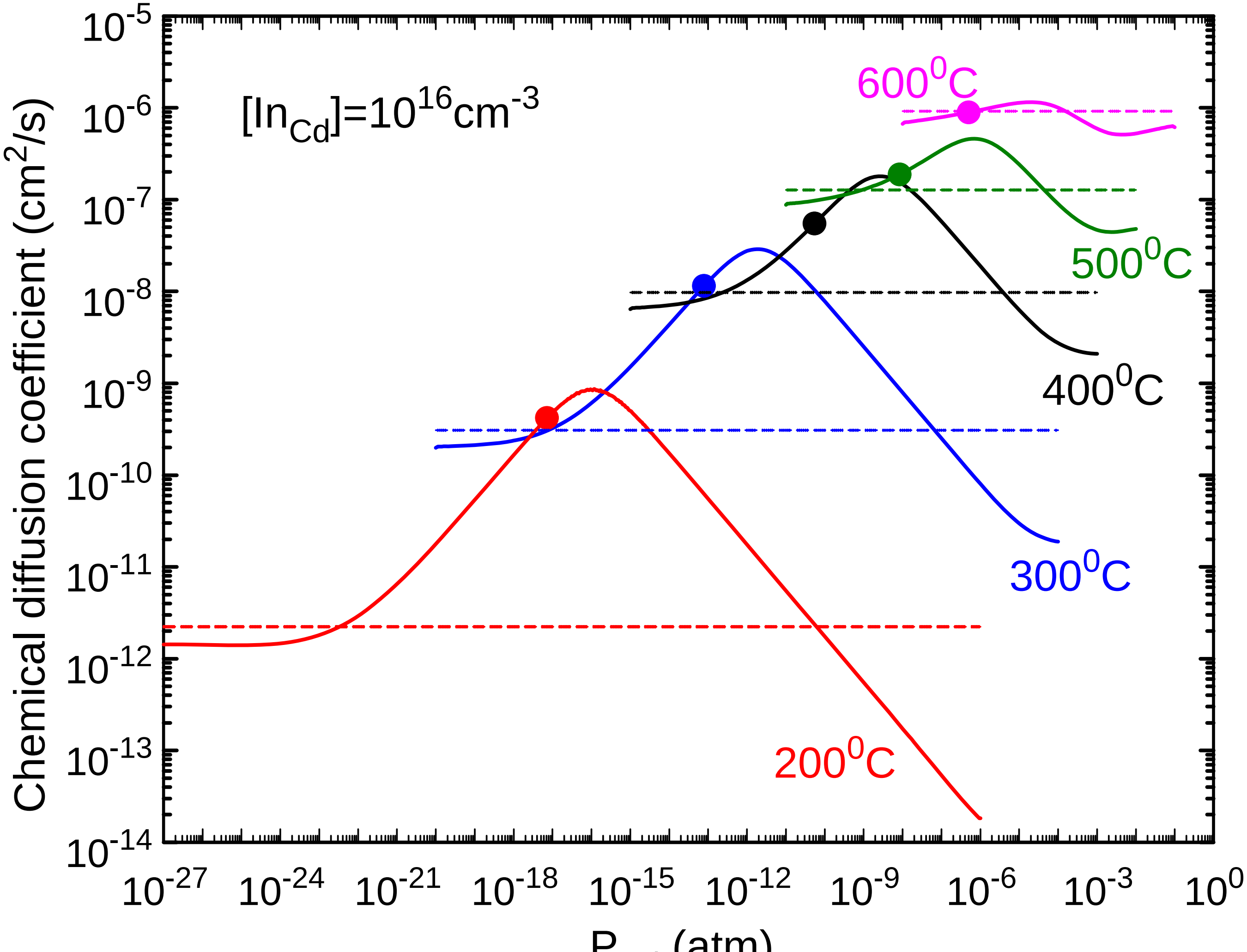
$$D(CdTe) = -\frac{J_\Delta}{\frac{d\Delta}{dz}} = \sum_{X,q} D_X^q \frac{X^q}{X^0} \left| \frac{dX^0}{d\Delta} \right|$$

$\Delta =$ stoichiometry deviation

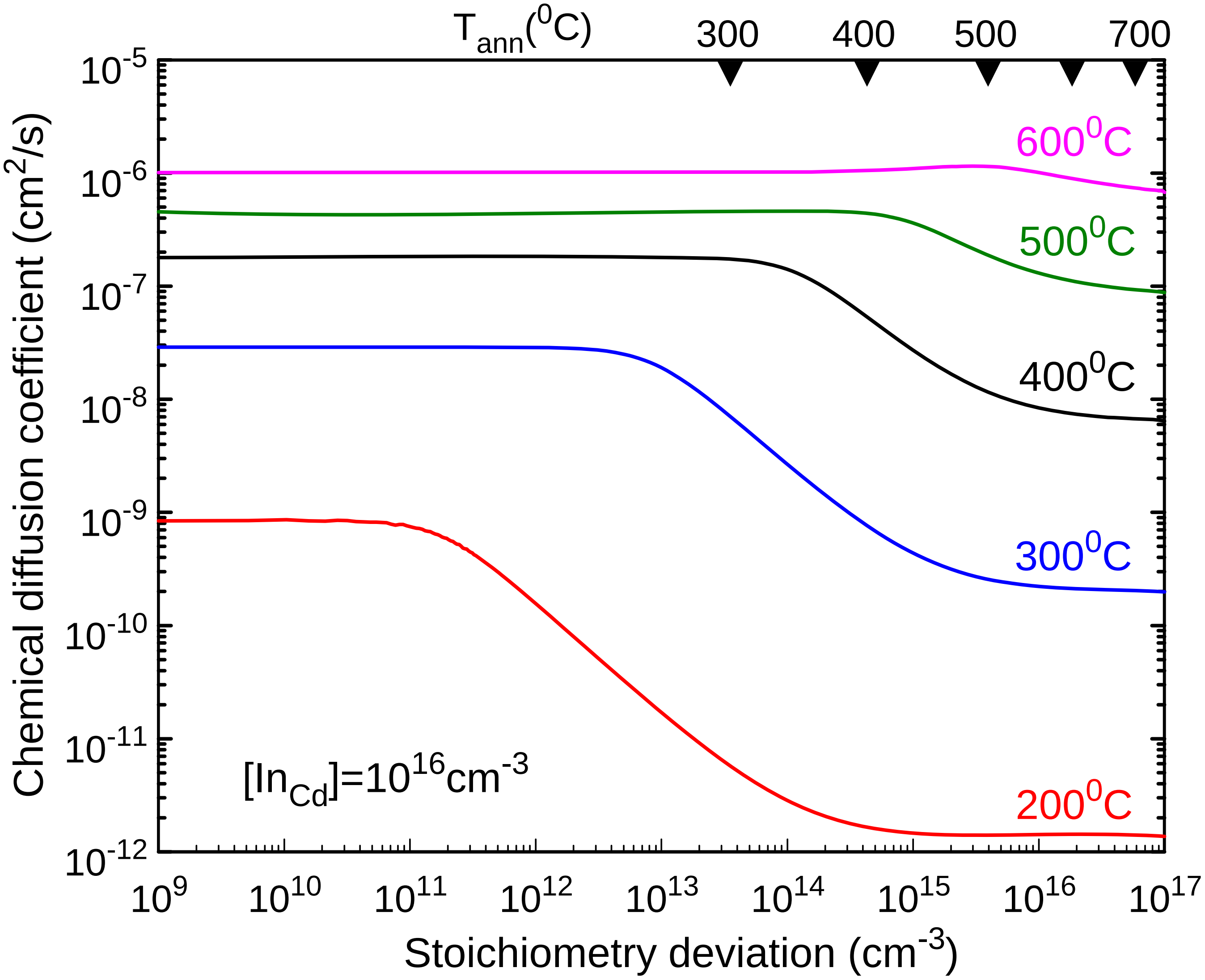
Enhanced low-temperature diffusion in CdTe:In near Te-saturation



Temperature scan of diffusion coefficient near Te-saturation



Diffusion enhancement at low stoichiometry deviation only



Conclusion

- Diffusion of charged point defects is significantly affected by induced electric field.
- Extrinsic doping enhances the diffusion of compensating native defects.
- Donor doping accelerates low-temperature relaxation of Cd vacancies in CdTe at low stoichiometry deviation.
- The profit of the enhanced diffusion for the preparation of detector-grade CdTe can be utilized, if slow cooling at medium temperature is performed.