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Fraunhofer Institute for Integrated Systems and Device Technology IISB

Impurity Diffusion and Activation: Ever Growing Challenges, Complexity, and Predictivity

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Contents

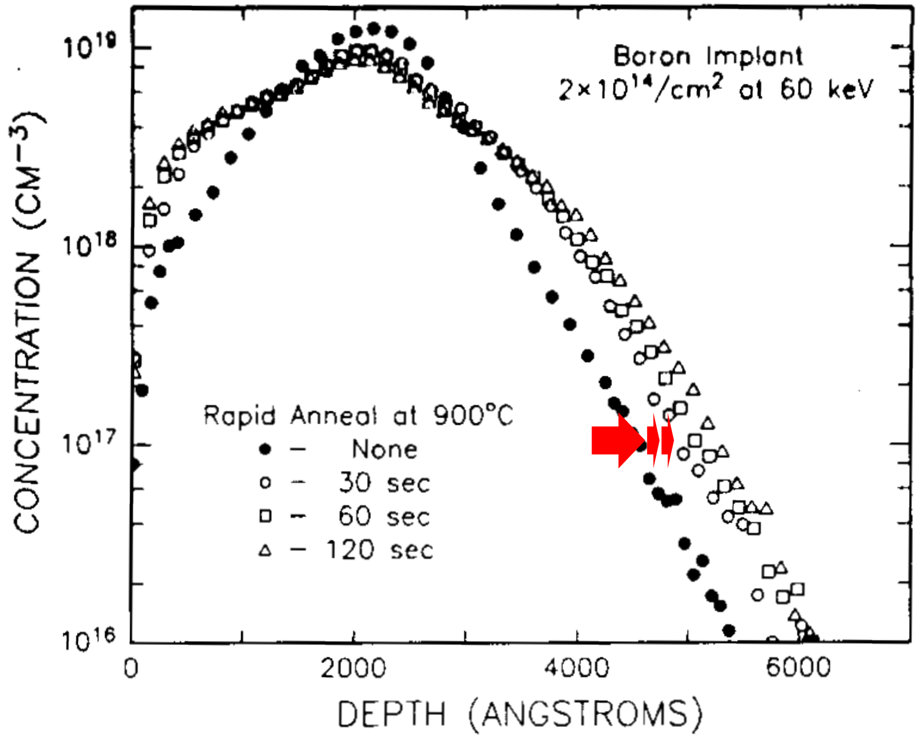
Motivation

- During the last 40 years continuing Power-Performance-Area-and-Cost (PPAC) scaling
  - Shallower profiles with higher concentrations after annealing at ever lower temperatures and shorter times
  - Transient enhanced diffusion and reduced activation highly undesirable
  - Subsequent European projects to understand, model and eventually reduce them
    - RAPID "Redistribution and Activation Phenomena in Integrated Circuit and Device Manufacturing" 1997 – 2000
    - FRENDTECH "Front-End Models for Silicon Future Technology" 2001 – 2004
    - ATOMICS "Advanced Front-End Technology Modeling for Ultimate Integrated Circuits" 2006 – 2009
    - ATEMOX "Advanced Technology Modeling for Extra-Functionality Device" 2010 – 2013
    - MUNDFAB „Modeling Unconventional Nanoscaled Device FABrication" 2020 – 2023
- Model development for power device processing brings additional challenges
  - Impurities like platinum for lifetime engineering
  - High-bandwidth materials like 4H-SiC as alternative to silicon
- As do quantum technology, spintronics, nanosized sensors, detectors and other unconventional electron devices

Implantation-enhanced diffusion

Phenomenology

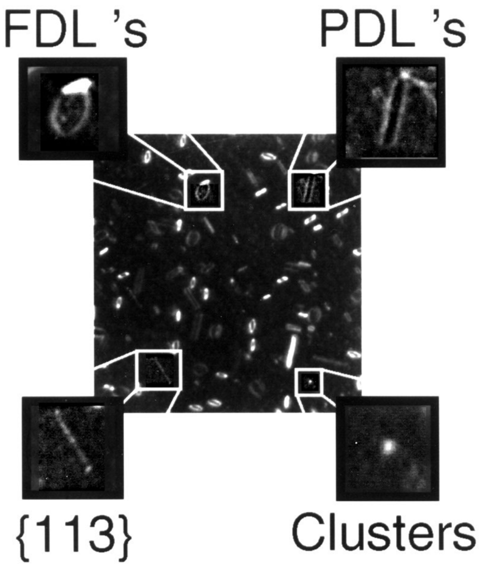
- After Rapid Thermal Annealing came into use, boron diffusion was found to decrease rapidly with annealing time
- Many explanations – mostly empirical or even wrong
- First association to the growth of extended self-interstitial clusters by Yudong Kim, a student of Massoud, Gösele and Fair in 1990
- Around about 1994 fist attempts to investigate the phenomenon in the framework of a European ESPRIT project
  - RAPID Redistribution and Activation Phenomena in Integrated Circuit and Device Manufacturing
  - P. Pichler (IIS-B), A. Claverie (CNRS), D. Tsoukalas (IMEL), A. Willoughby (Univ. Southampton), N.E.B. Cowern (Philips)
- Third attempt successful (1997 – 2000)



E. A. Michel et al. Appl. Phys. Lett. 50(7), 416 (1987)

Available experiments for silicon

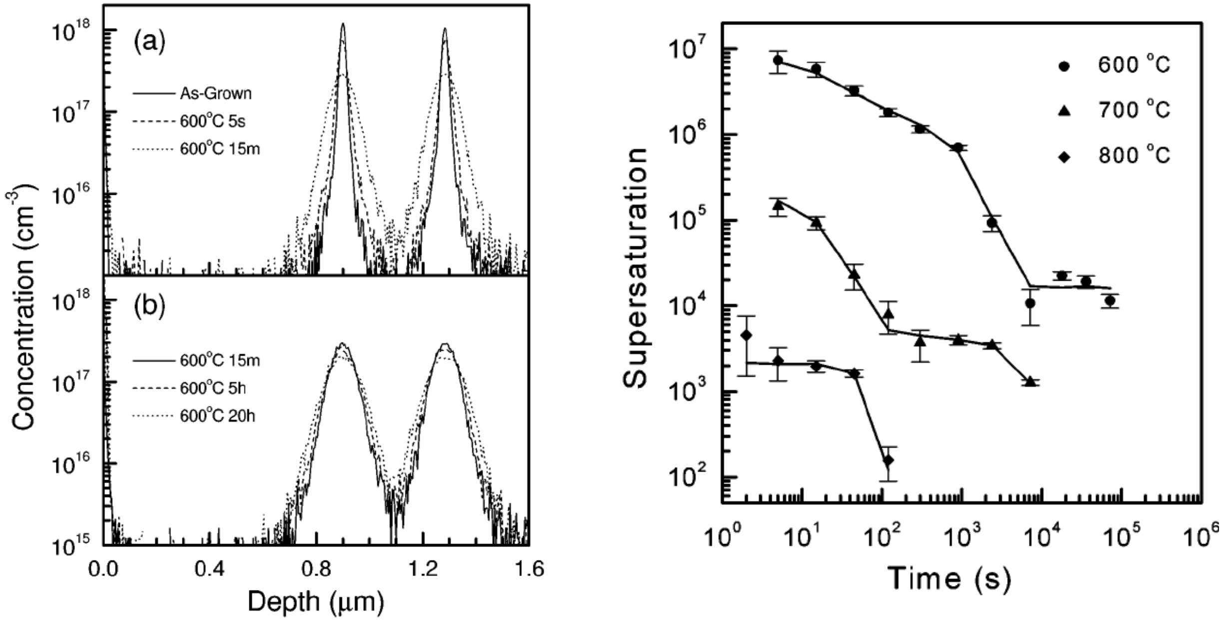
TEM observation of the growth of extended defects identified as self-interstitial agglomerates



Bonafos, Claverie, Eaglesham, Gossmann, Jones, Laânab, Li, Seibt, Stolk, Takeda, etc. all around 1994 to 1998

Review by A. Claverie et al., Appl. Phys. A 76, 1025 (2003)

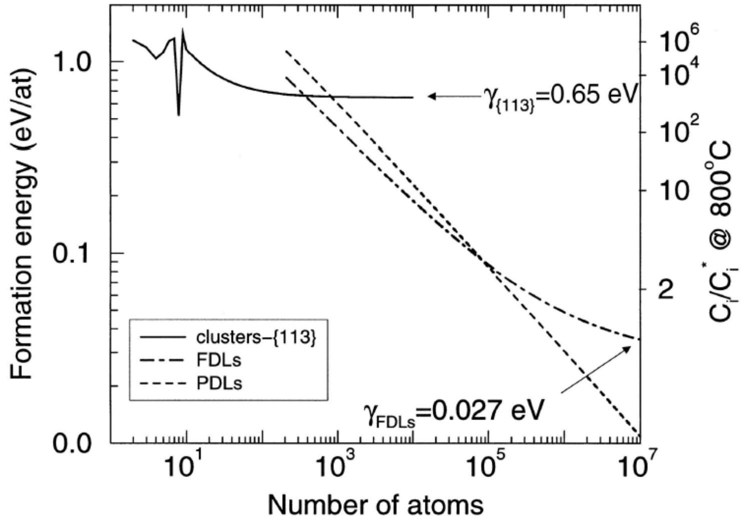
Self-interstitial oversaturation from the diffusion of boron marker layers after a surface-near silicon implantation

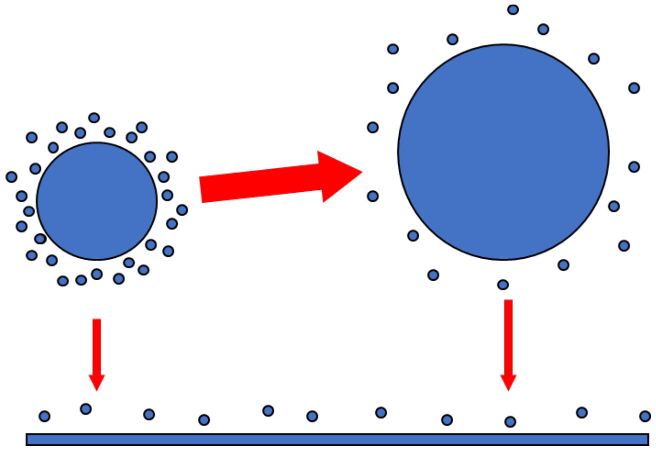


N.E.B. Cowern et al., Phys. Rev. Lett. 82, 4460 (1999)

Available experiments for silicon

- Each of the self-interstitial agglomerates maintains a cloud of self-interstitials in its vicinity
- The higher the formation energy, the higher the self-interstitial concentration in the cloud in equilibrium with the extended defect
- Smaller extended defects are energetically less favorable than bigger defects
- Net flux of self-interstitials from small to big clusters ⇨ growth of big clusters at the expense of the small ones ⇨ Ostwald ripening
- Multi-species system to be considered since the formation energy reduces from small clusters via {113} defects and small faulted dislocation loops to big perfect loops
- Transient diffusion determined by the mean oversaturation of self-interstitials
- Finally, dissolution of all self-interstitial agglomerates because of the loss of self-interstitials to the surface





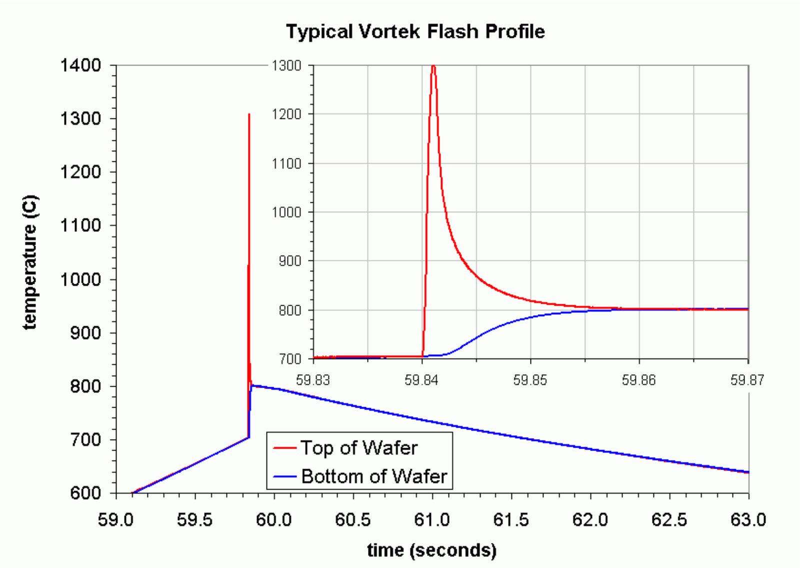
A. Claverie et al., Appl. Phys. A 76, 1025 (2003)

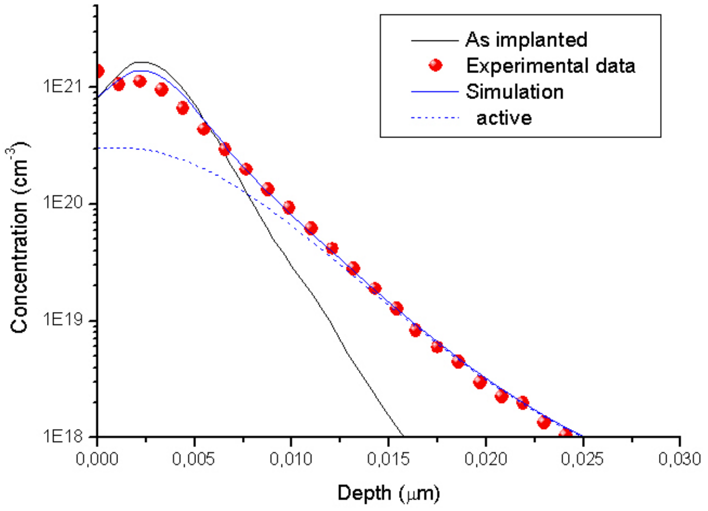
Modeling

- Modeling Ostwald requires simulation of the interaction of all kinds of self-interstitial clusters

$$I_n + I \rightleftarrows I_{n+1}$$

- For every-day simulations:
  - Simulate 1000 equations and more (Ortiz et al.) – example to the right
  - Simulate equations for the small clusters and a Fokker-Planck equation for the big ones (E. Lampin et al., still lives as FRENDTECH model in Sentaurus Process
  - Drastically reduced to 3 equations for small clusters plus 2-moment models for {113} defects (C. Zechner et al.) and dislocation loops (N. Zographos et al.) – Full cluster model in Sentaurus Process
  - Extended further 2015 by F. A. Wolf at Bosch to separate faulted and perfect DLs for the high thermal budgets needed for PV processing

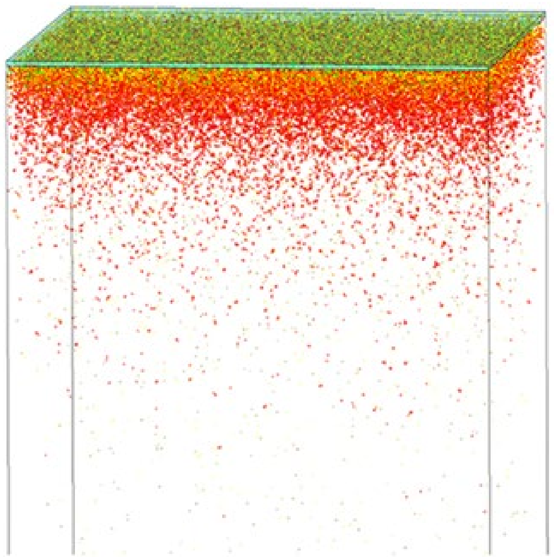


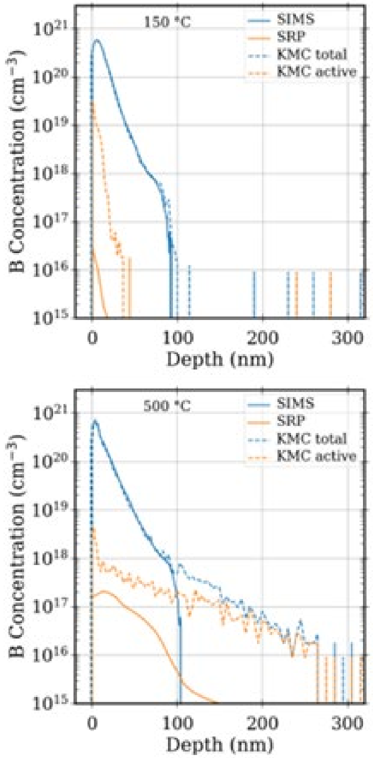


P. Pichler et al., DDF 258-260, 510 (2006)

In the meanwhile, …

- In 3D sequential integration schemes, active layers are stacked on top of each other
- Thermal budget drastically limited (< 500 °C) in order not to degrade lower layers when processing the topmost layer
- Models for such processes were a main point of research in the H2020 project MUNDFAB „Modeling Unconventional Nanoscaled Device FABrication“ (2020-2023)
- Implantation at 200 to 500 °C as a possible method to improve activation
- Kinetic Monte Carlo simulation within Sentaurus Process to get a complete picture of ion implantation with damage production and the concurrent annealing and diffusion processes.
- Recalibration of interstitial boron properties required to improve agreement between simulation and experiments





S. Mundinar et al., presentation in Symposium M, E-MRS Spring Meeting 2023

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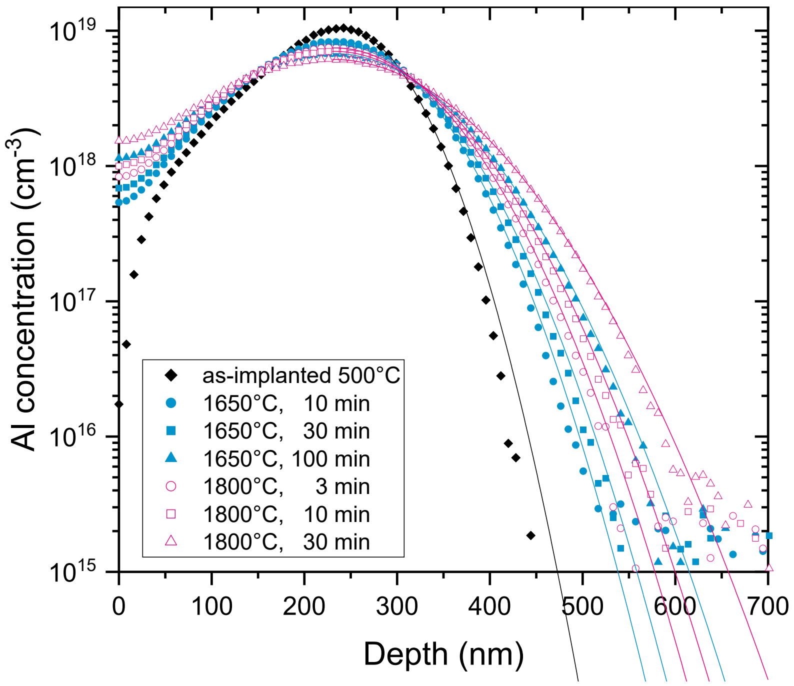
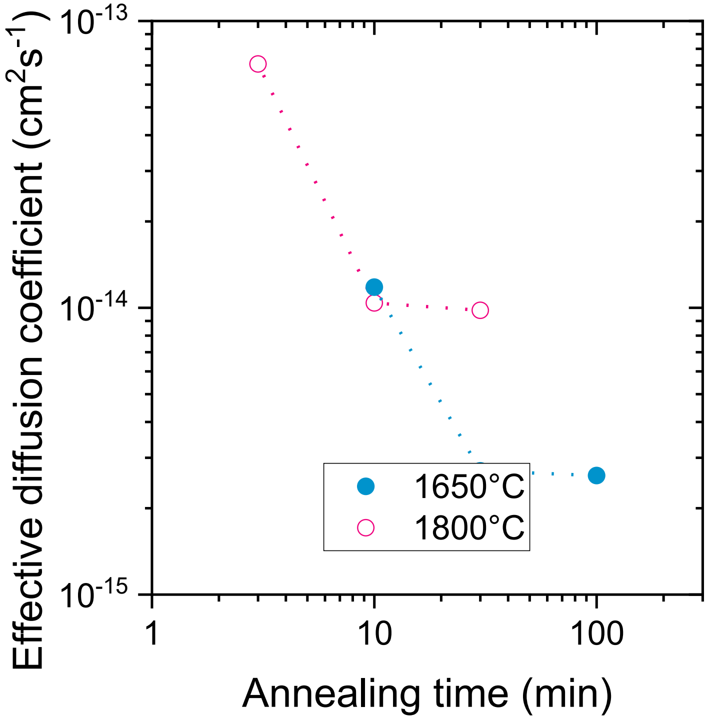
And there are also other materials like SiC

- Activation of aluminum implanted into 4H-SiC requires annealing above 1600 °C
- Diffusion in such samples could be well described by Gaussian diffusion
- Enhanced diffusional broadening observed for the shortest annealing time
- Ion implantation at 500 °C leads to a reduced broadening for the shortest annealing time
- But what is the mechanism?





K. L. Mletschnig, P. Michalowsi and P. Pichler, presented at the ICSCRM conference 2023

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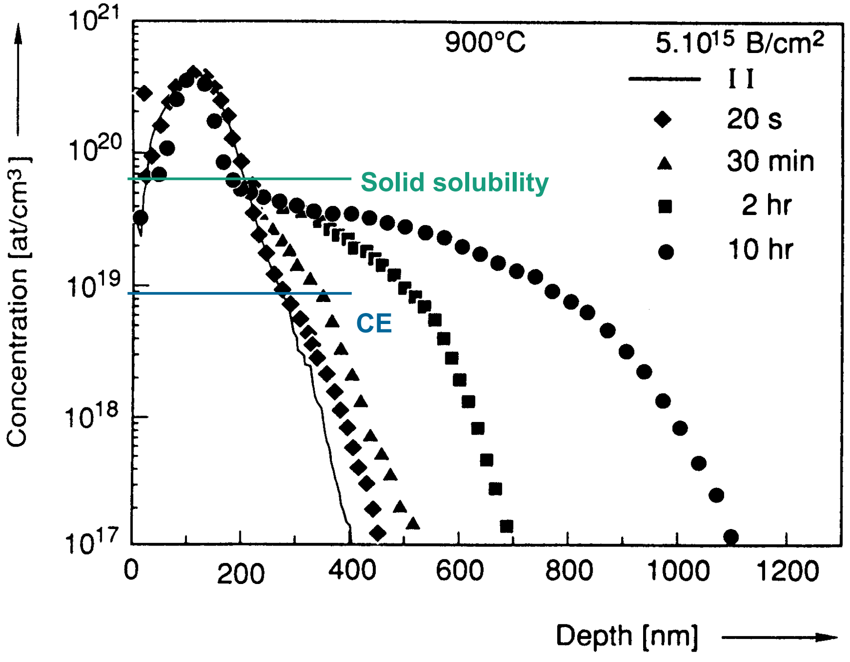
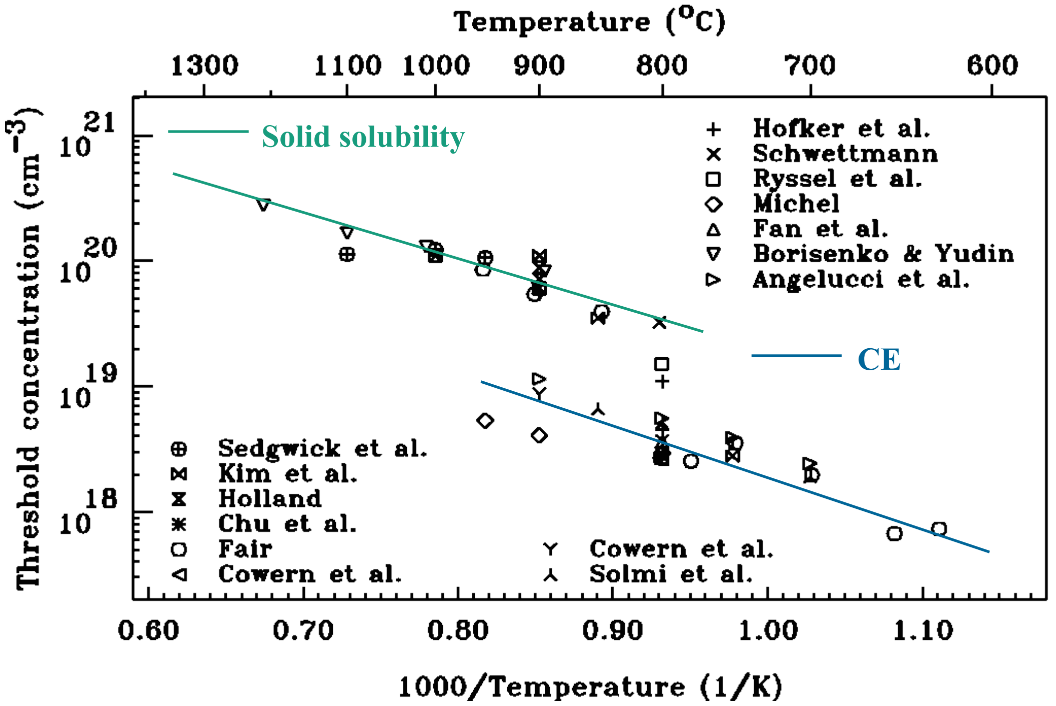
Phenomenology

During post-implantation annealing, boron diffusion only observed below a concentration which increases with time to the solid solubility value, the immobile boron was electrically inactive



N.E.B. Cowern et al., J. Appl. Phys. 68, 6191 (1990)

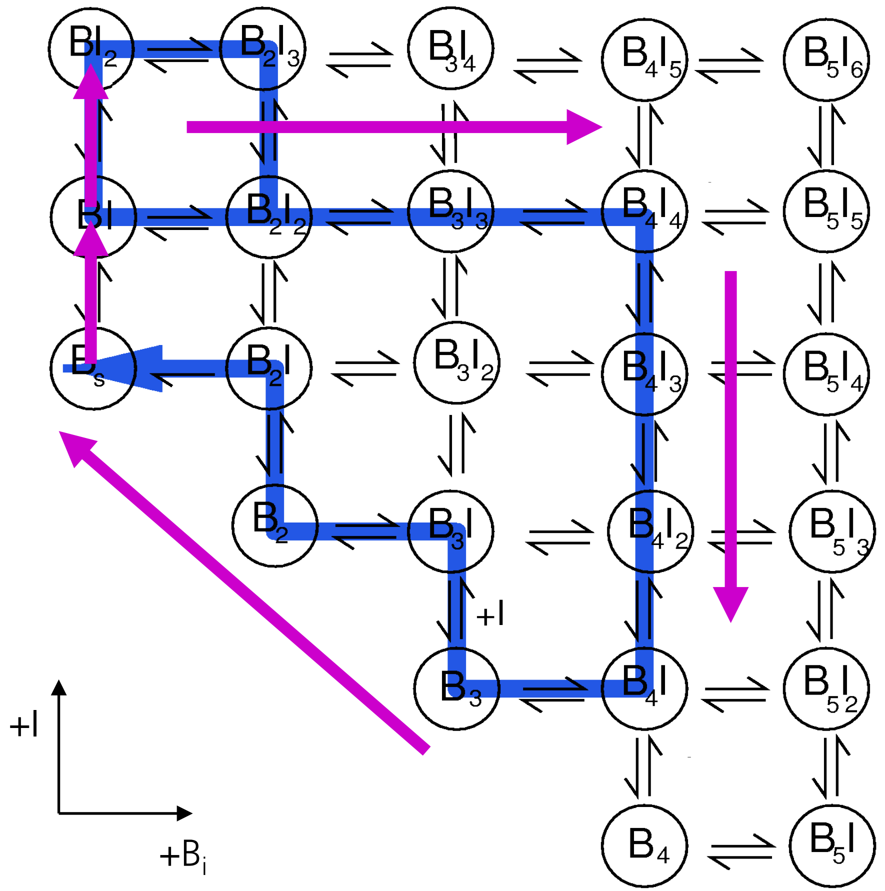


P. Pichler, Mat. Res. Soc. Symp. Proc. 717, C3.1.1 (2002)

Boron activation

Boron-interstitial clusters

- Many experiments involving boron delta-doped layers made clear that the immobile boron complexes also contain self-interstitials (Eaglesham, Haynes, Jones, Lilak, Mannino, Solmi, Stolk, …)
- First models predicting reactions between self-intersitials I, boron interstitials BI and so-called Boron-Interstitial-Clusters (BICs) suggested 1997 by Pelaz et al. and Caturla et al.
- Required BIC parameters from atomistic simulations (Zhu, Windl, Sadigh, Jeong, Oshiyama)
  which resulted in part in significantly different formation energies
- Taken up in RAPID soon after
- Problem then: How to calibrate the BIC parameters on the basis of experimental data?



Calibration efforts

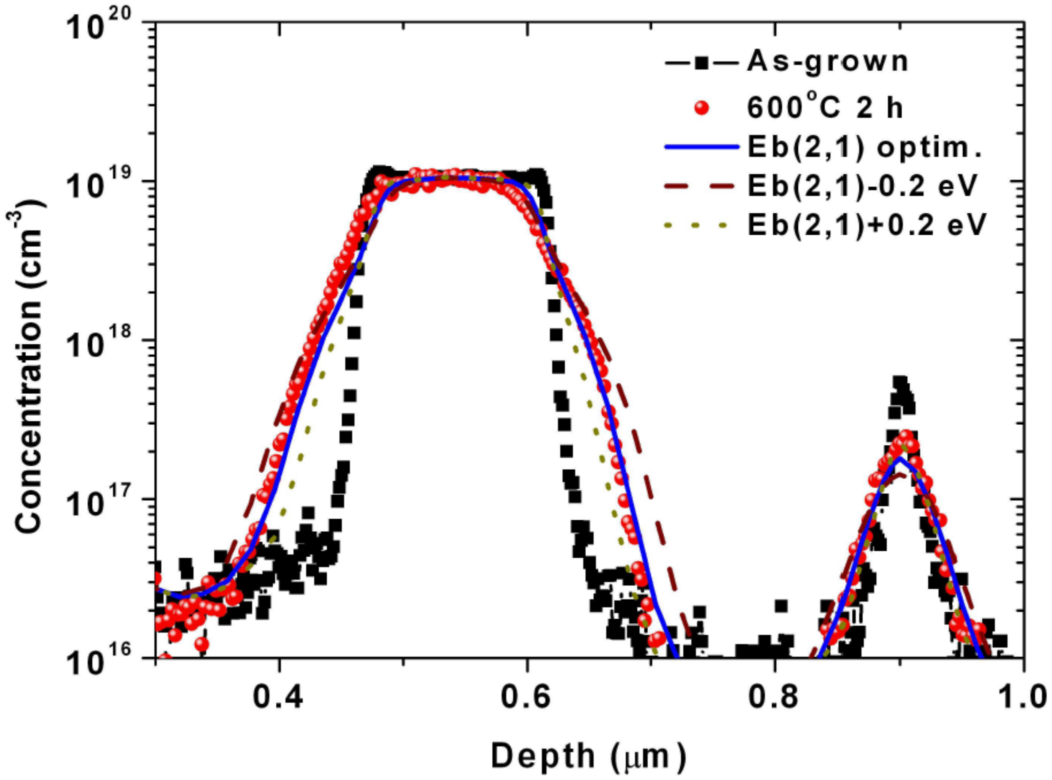
FRENDTECH (2001-2004)

- Highly-doped boron layers and BIC formation induced at low temperatures by surface near silicon implants
- Identification of spectroscopic signatures of BICs by ab-initio simulations (P. Déak, A. Gali). Unfortunately, none of the signatures could be found experimentally
- Calibration of some BICs like B_4I_2 allowed to reproduce profiles after spike and flash annealing

In MUNDFAB, boron activation during ion implantation at elevated temperatures reappeared as an issue in KMC simulations:

- Ion implantation generates some 40 vacancies per implanted boron atom ⇨ boron interstitials become all substitutional
- Measured activation significantly lower

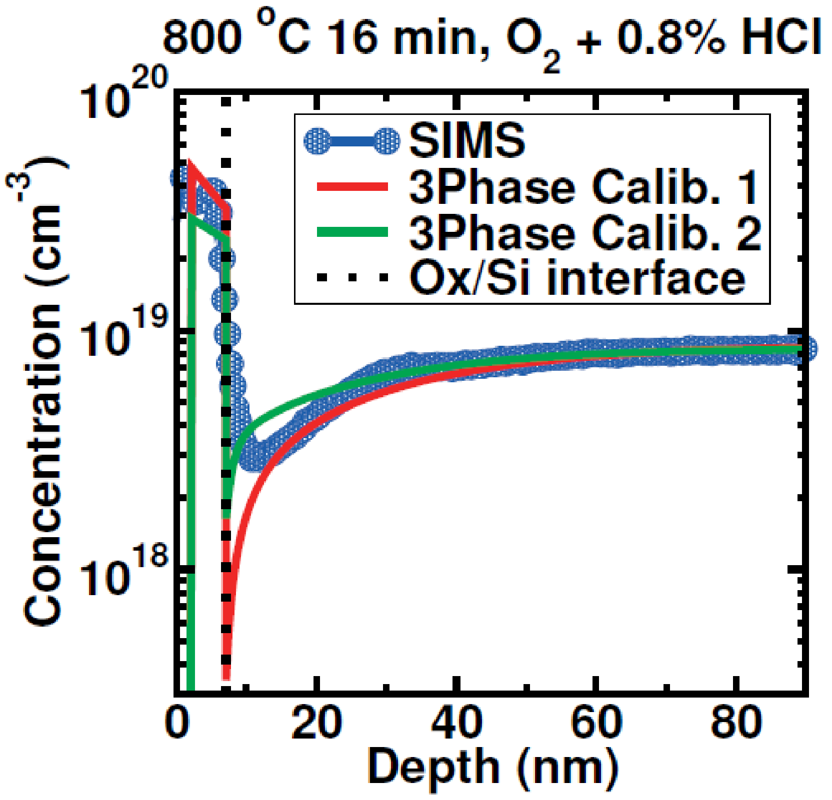
For SiC and UWBG materials complication due to compensating defects and deep dopant levels



P. Pichler et al., IEDM Techn. Digest, 967 (2004)

Calibrating pMOS threshold voltage in ATHENIS (2008-2011)

- Our task in ATHENIS: Calibration of the threshold voltage of a 0.35 µm CMOS process of ams AG
- Boron known to segregate preferentially into the oxide during an oxidation process
- Threshold voltage of the pMOS transistor found to be determined by a very special distribution of n-type and p-type dopants in the channel and to be very sensitive to the boron concentration in the channel
- This allowed a calibration of the three-phase segregation model implemented in Sentaurus Process in the temperature range from 800 to 900 °C

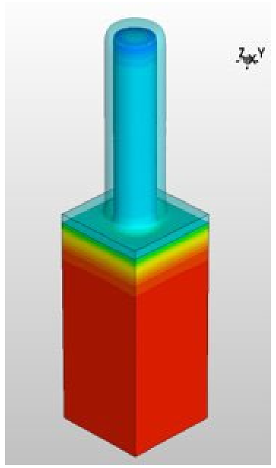


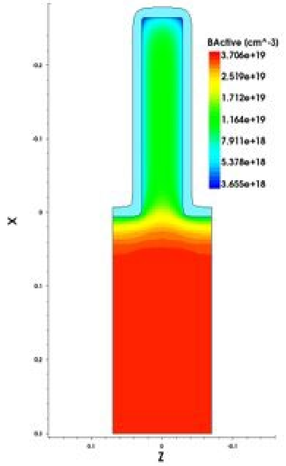
S. Koffel et al., Phys. Status Solidi C 11, 12 (2014)

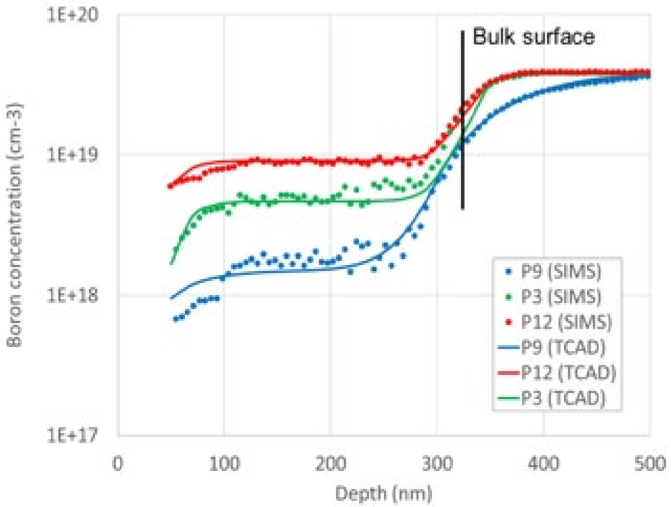
Boron segregation

Oxidation of vertical nanowires in MUNDFAB

- Vertical junctionless gate-all-around nanowire transistors fabricated by CNRS-LAAS used as demonstrator in MUNDFAB
- Sacrifical oxidation for thinning of the nanorods and also to remove damage introduced during etching
- During oxidation, a considerable part of the boron doping segregates to the growing oxide
- New SIMS methodology developed by Paweł Michałowski of Łukasiewicz - Instytut Mikroelektroniki i Fotoniki to characterize the boron concentration in the nanorods
- Segregation coefficients had to be recalibrated to give lower residual concentrations



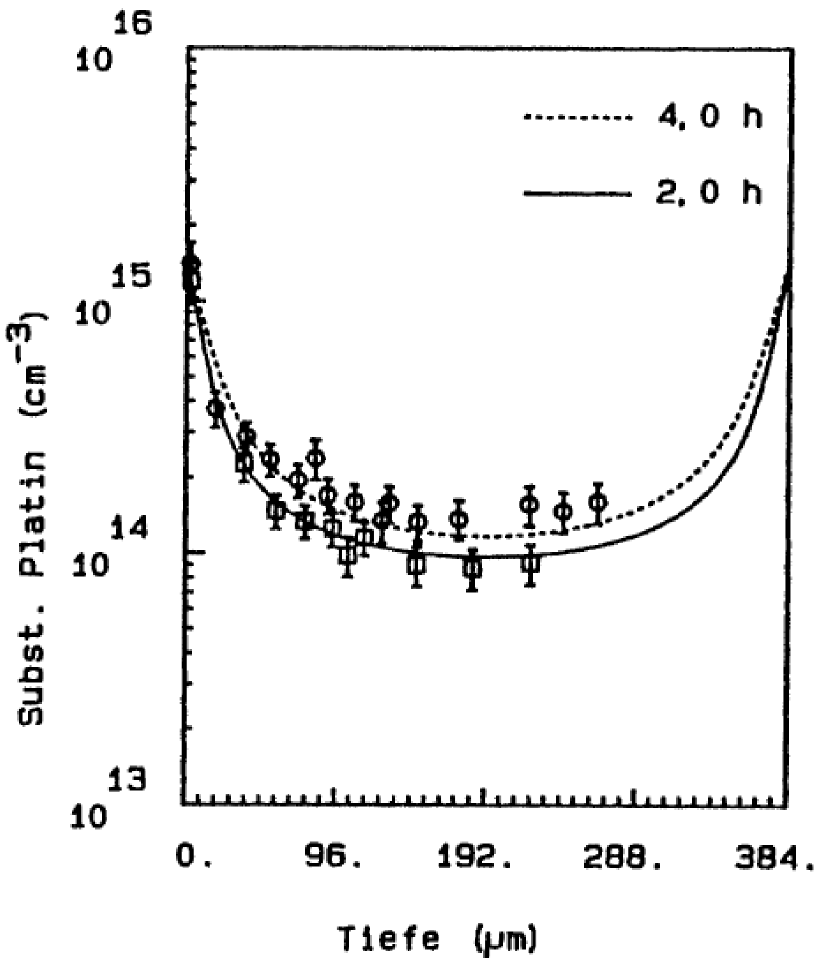




C. Rossi et al., H2020 MUNDFAB (2023)

Early work by H. Zimmermann (1985-1991)

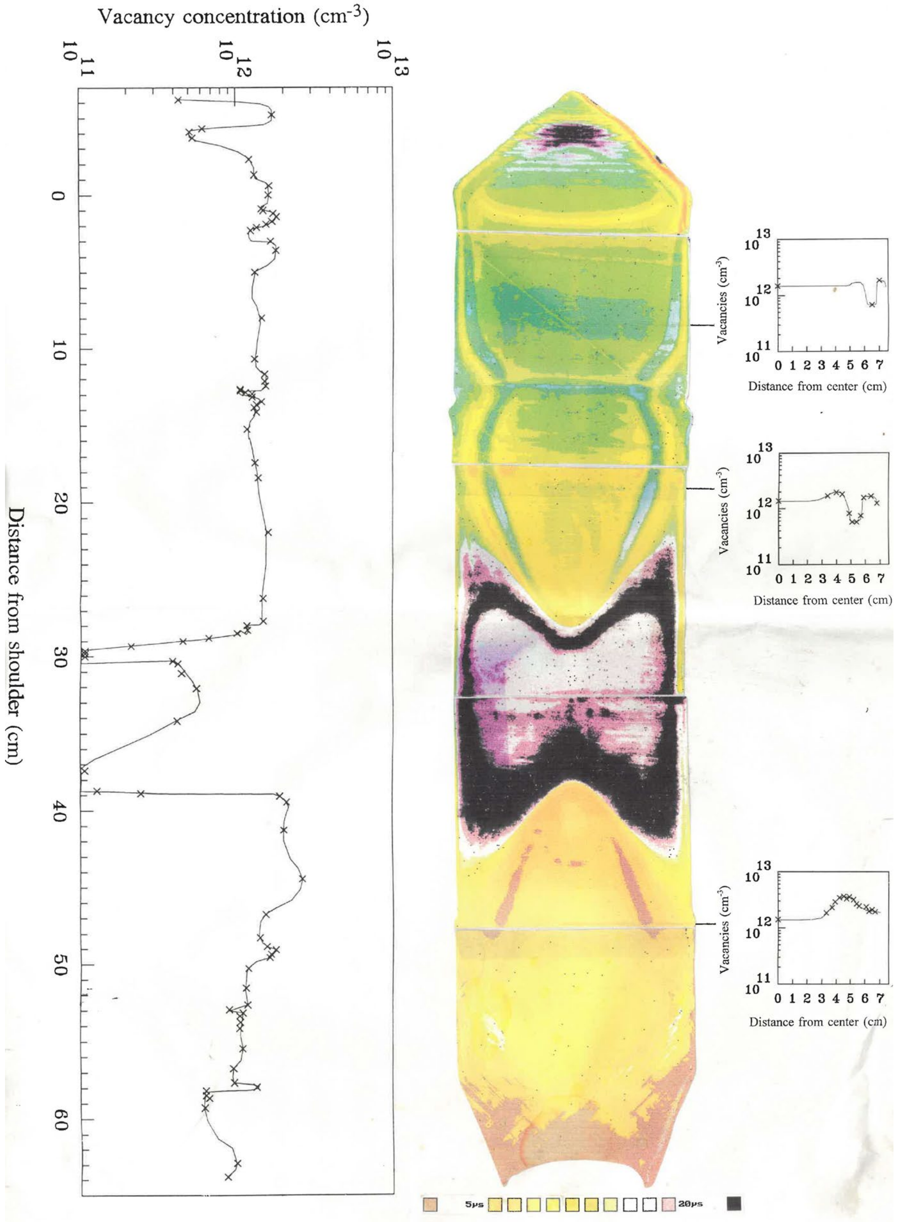
- Platinum used for lifetime engineering in power semiconductors
- Rapid interstitial platinum diffusion from deposited layers
- Change from substitutional to interstitial site require interactions with intrinsic point defects:
  - $Pt_i + V \rightleftharpoons Pt_s$ – Frank-Turnbull mechanism
  - $Pt_s + I \rightleftharpoons Pt_i$ – Kickout mechanism
- Vacancies are supplied and self-interstitials recombine at the surfaces ⇨ nearly symmetric U-shaped profiles
- As a side-product:
  Methodology found to characterize the concentration of vacancies via short-time platinum diffusion



H. Zimmermann, PhD thesis, Univ. Erlangen (1991)

Platinum diffusion
Platinum to characterize vacancy concentrations

- Platinum diffusion from a sputtered source at about 730 °C
- Platinum interstitials decorate the vacancies
- Measured by DLTS or via lifetime measurements
- Used by MEMC (B. Falster and V. V. Voronkov) to investigate and optimize point-defect introduction during crystal growth and oxygen precipitation
- Common projects with MEMC from 1992 to 2001 with 2 PhD thesis
  - M. Jacob (1996)
  - F. Quast (2001)

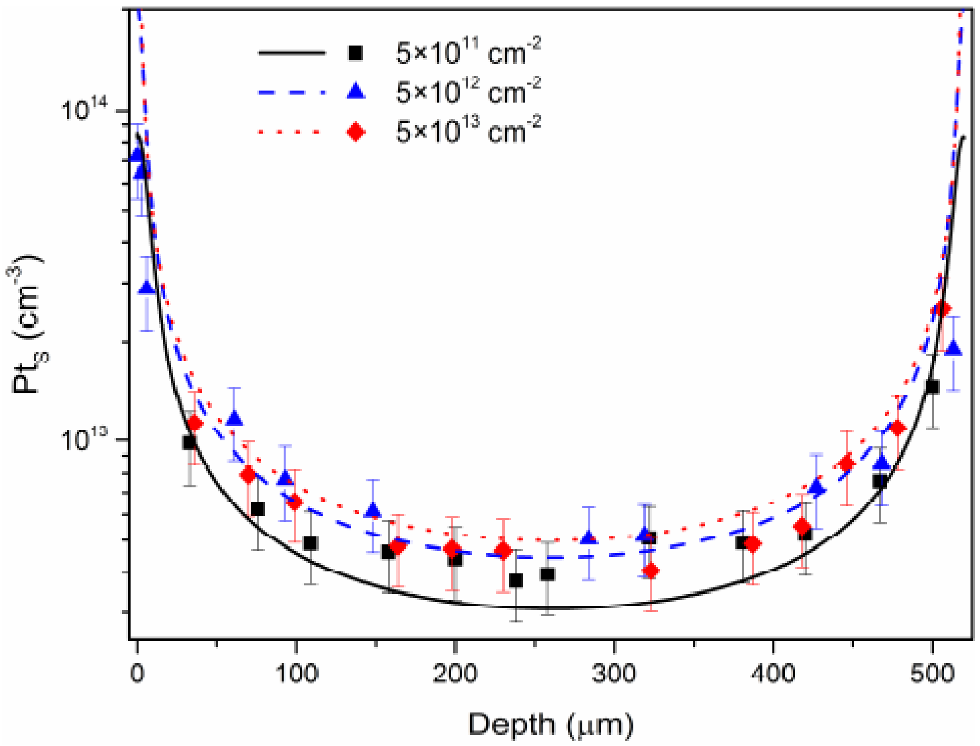


M. Jacob, Project with MEMC (1995)

Platinum diffusion

Platinum for lifetime engineering

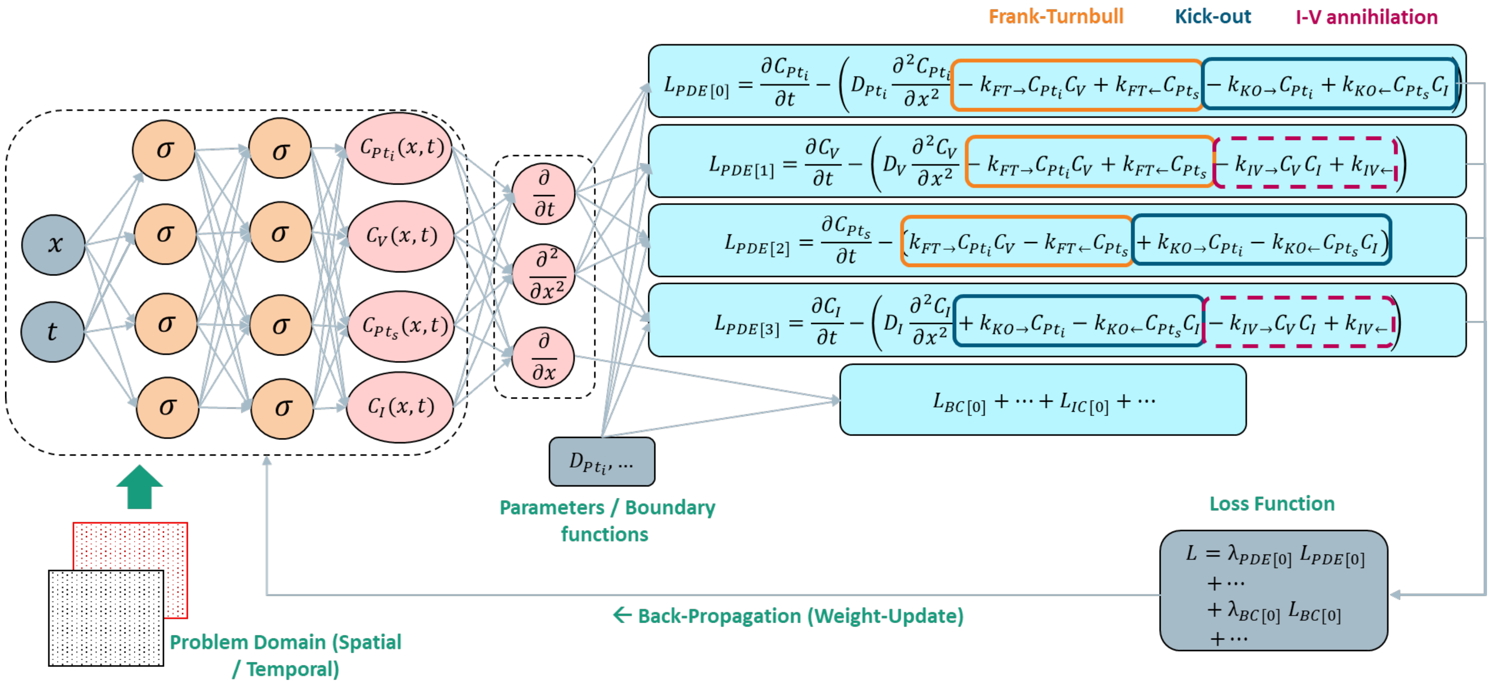
- Focus at Infineon changed to
  - Implanted platinum
  - Single-sided gettering of platinum by a highly doped phosphorus layer (phosphorus-diffusion gettering, PDG)
- Requires in addition to models for platinum to include models for
  - Ostwald ripening of self-interstitial agglomerates
  - Clustering of platinum atoms
- Common projects with Infineon from 2011 to 2019 with 2 PhD thesis
  - E. Badr (2017)
  - A. Johnsson (2019)
- Allowed also to determine basic properties of intrinsic point defects
- Review available as A. Johnsson et al., Phys. Status Solidi A 219, 2100462 (2022)

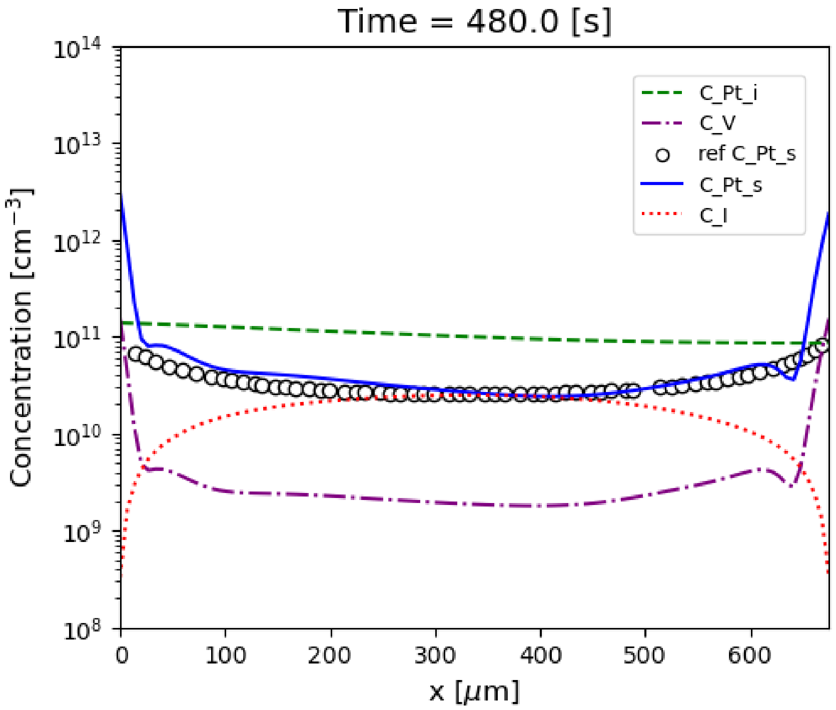


E. Badr, P. Pichler, G. Schmidt, Solid State Phenom. 242, 258 (2016)

Solution of the platinum diffusion equations

- In the past: Discretization and numerical solution of a set of continuity equations
- Possibly in future: Trainung of Neural Networks with physics and data





P. Zinesi, P. Brendel, C. Rossi, S. Mundinar (unpublished)

Conclusions

- Many transient phenomena in impurity diffusion and activation can be quantitatively reproduced in silicon and silicon-rich SiGe
- This does not mean that they are completely understood
- Going to lower temperatures, shorter processing times for nanoelectronics often requires to take a step back
- Materials like SiC and other Ultra-Wide-Bandgap materials bring new challenges particularly for dopant activation

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