Diffusion in Semiconductors via PINNs

General idea

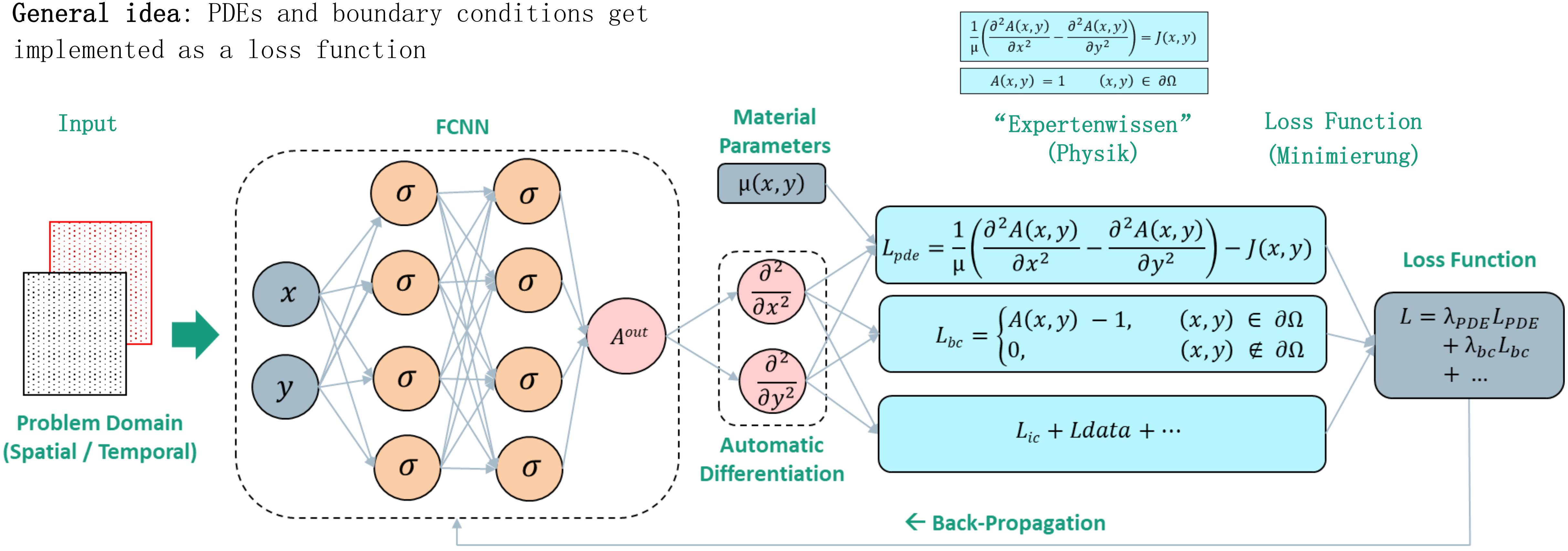
- Diffusion in semiconductors is an extremely relevant topic:
  - Dopants are implanted and annealed and will diffuse during this process
  - During annealing diffusion can repair crystalline damage
  - Silicides are used to create good ohmic contacts, they are created by diffusing metal into semiconuctor material

- Diffusion processes can be simulated by diffusion-reaction equations and appropriate boundary conditions
- Diffusion-reaction equations are partial differential equations (PDEs) that incorporate different ways for different particles to diffuse or react with other kinds of particles

Diffusion of Defects via PINNs

Physics-Informed Neural Networks (PINNs)

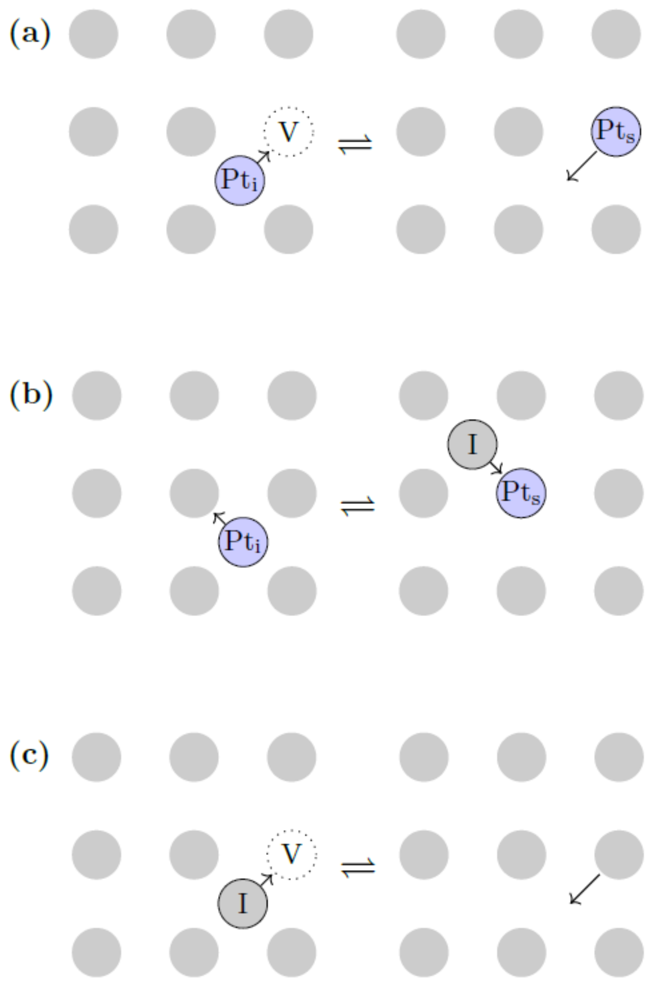
- **General idea:** PDEs and boundary conditions get implemented as a loss function



What has been done

Diffusion von Pt in Si

- Intrinsic point defects in Si: Vacancies (V) and Self-Interstitials (I)
- Pt can take substitutional (s) or interstitial (i) position
- Different possible processes that can lead to the diffusion of of Pt:
  - Frank-Turnbull Mechanism (a)
  - Kick-out Mechanism (b)
  - Recombination (c)
- In total 4 PDEs for concentrations of Pt_s, Pt_i, I und V
- Concentration of Pt shows a characteristic U-Shape during the annealing process



Reaction-Diffusion Model of SiC Silicidation

- **Basic Model [1]:**

$$\frac{\partial C_{Ni}}{\partial t} = \frac{\partial}{\partial x}\left(D^* \frac{\partial C_{Ni}}{\partial x}\right) - k_{11} C_{Ni} C_{SiC} - k_{21} C_{Ni} C_{NiSi}$$

$$\frac{\partial C_{SiC}}{\partial t} = \frac{\partial}{\partial x}\left(D^* \frac{\partial C_{SiC}}{\partial x}\right) - k_{11} C_{Ni} C_{SiC} - k_{12} C_{NiSi} C_{SiC}$$

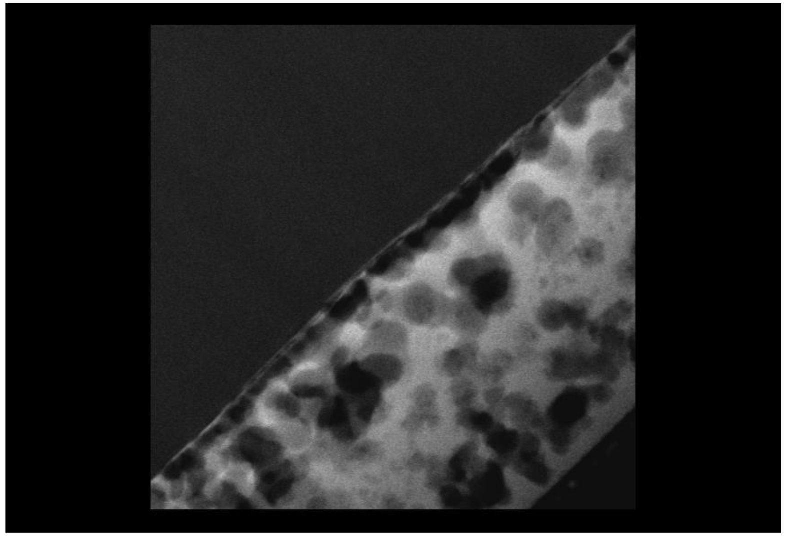
$$\frac{\partial C_{C}}{\partial t} = \frac{\partial}{\partial x}\left(D^* \frac{\partial C_{C}}{\partial x}\right) + k_{11} C_{Ni} C_{SiC} + k_{12} C_{SiC} C_{NiSi}$$

$$\frac{\partial C_{NiSi}}{\partial t} = k_{11} C_{Ni} C_{SiC} - k_{21} C_{Ni} C_{NiSi}$$

$$\frac{\partial C_{NiSi_2}}{\partial t} = k_{12} C_{SiC} C_{NiSi}$$

$$\frac{\partial C_{Ni_2Si}}{\partial t} = k_{21} C_{Ni} C_{NiSi}$$

- **Additional Conditions:**
  - Boundary conditions
  - Initial conditions



[1] Aleksandrov et al., Semiconductors 43, 885 (2009)

AI - Methods

Physics-Informed Neural Network (PINN)	Optimizing a Discrete Loss (ODIL)	Kolmogorov-Arnold Networks (KANs)
https://github.com/lululxvi/deepxde	https://github.com/cselab/odil	https://github.com/KindXiaoming/pykan https://github.com/Blealtan/efficient