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FORMATION OF DISLOCATIONS IN HIGHLY DOPED N-TYPE CZOCHRALSKI SILICON

L. Stockmeier[1], M. Zschorsch[1,2], J. Friedrich[1,2], L. Lehmann[3]
[1] Fraunhofer THM, Am St.-Niclas-Schacht 13, 09599 Freiberg, Germany
[2] Department Crystal Growth, Fraunhofer IISB, Schottkystr. 10, 91058 Erlangen, Germany
[3] Siltronic AG, Berthelsdorfer Straße 113, 09599 Freiberg, Germany

Motivation

Background
Highly doped Czochralski (CZ) silicon (Si) material is used as substrate for fabricating n/n+ and p/p+ epitaxial structures in integrated circuits (ICs) [1]

Principle of the CZ growth process

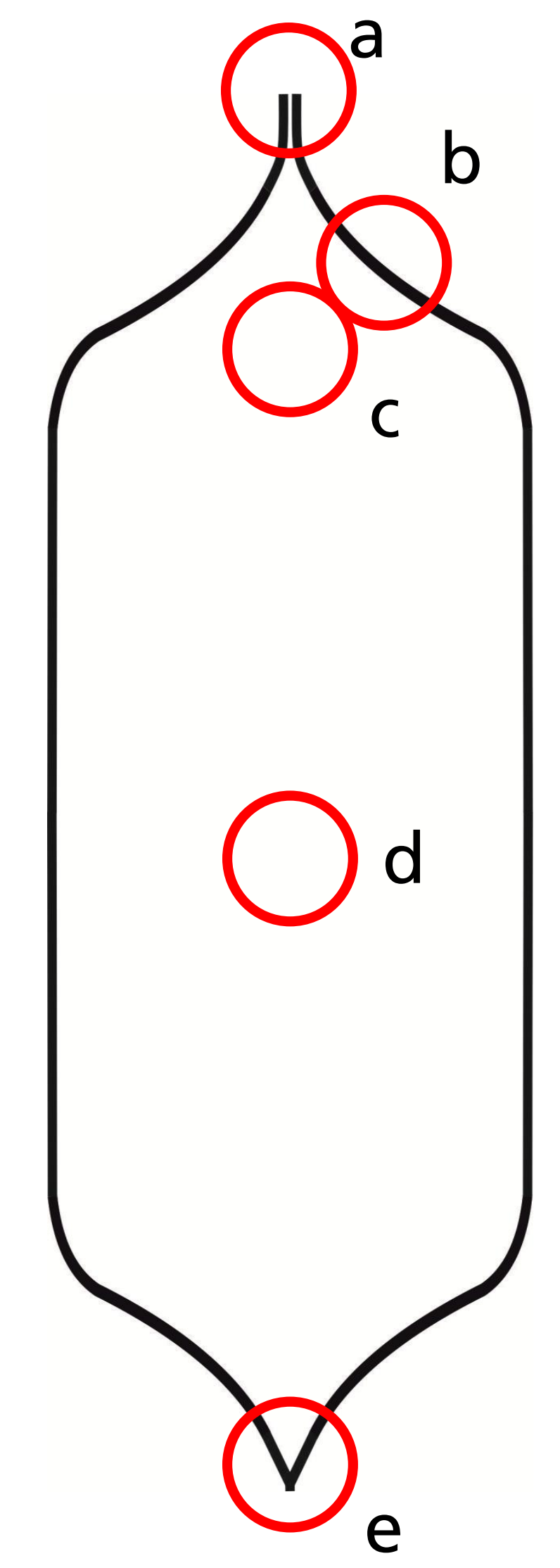
- Seeding and thin neck pulling by Dash method
- Diameter enlargement (cone step)
- Growth of cylindrical body
- Growth of end cone

Main challenges

- Dislocations are unwanted because they can lead to a polycrystalline structure
- Standard characterization methods are sometimes problematic on highly doped silicon

Aim of this work:
→ Scientific understanding of the dislocation formation and evaluation of characterization methods for highly doped silicon

Dislocations in CZ Silicon



Sketch of Czochralski crystal

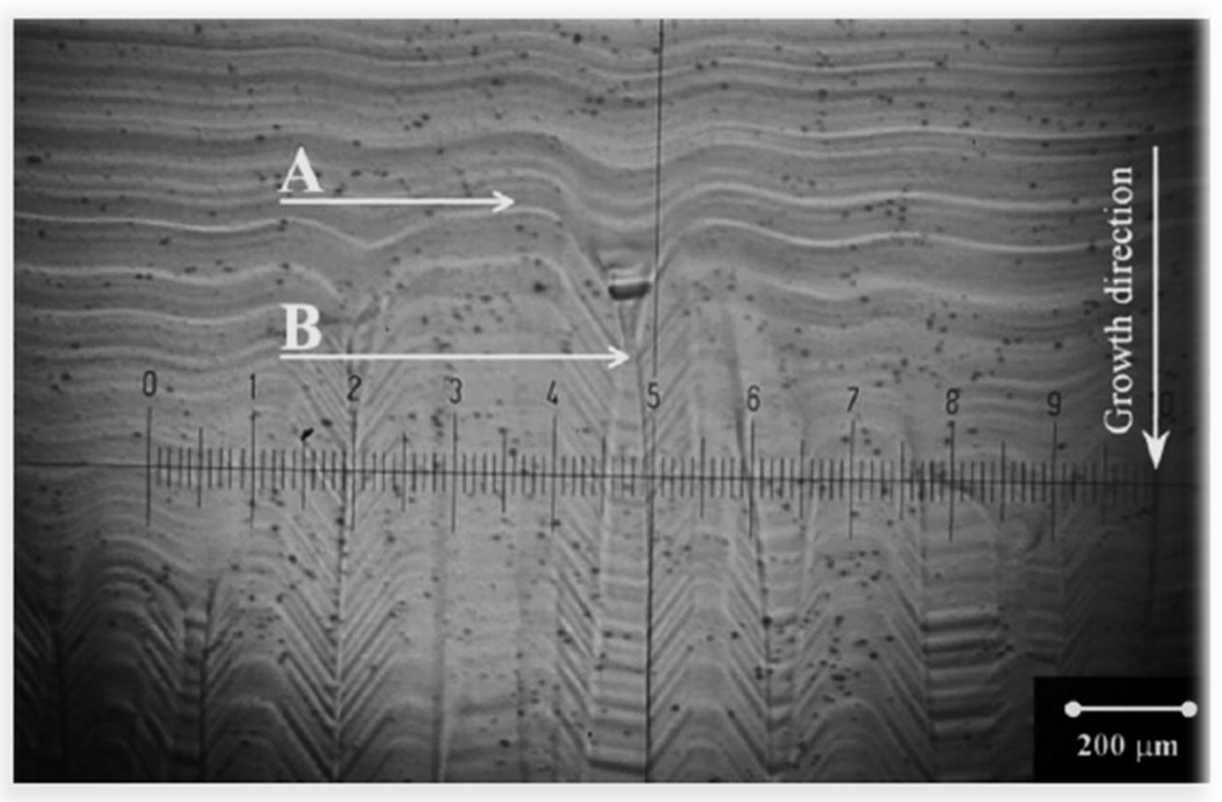
Possible dislocation origins

a. Seed
b. Cone edge
c. Cone center
d. Crystal rod
e. Cone end

Possible reasons for dislocations

1. Thermal stress (maximum at crystal edge)
2. Constitutional supercooling
3. Agglomeration of point defects
4. Lattice misfit (between undoped seed and highly doped crystal)
5. Thermal shock (at contact of seed with Si melt and at detachment of crystal from Si melt)
6. Embodiment of particles
7. Multiplication of dislocations

Parameters of interest

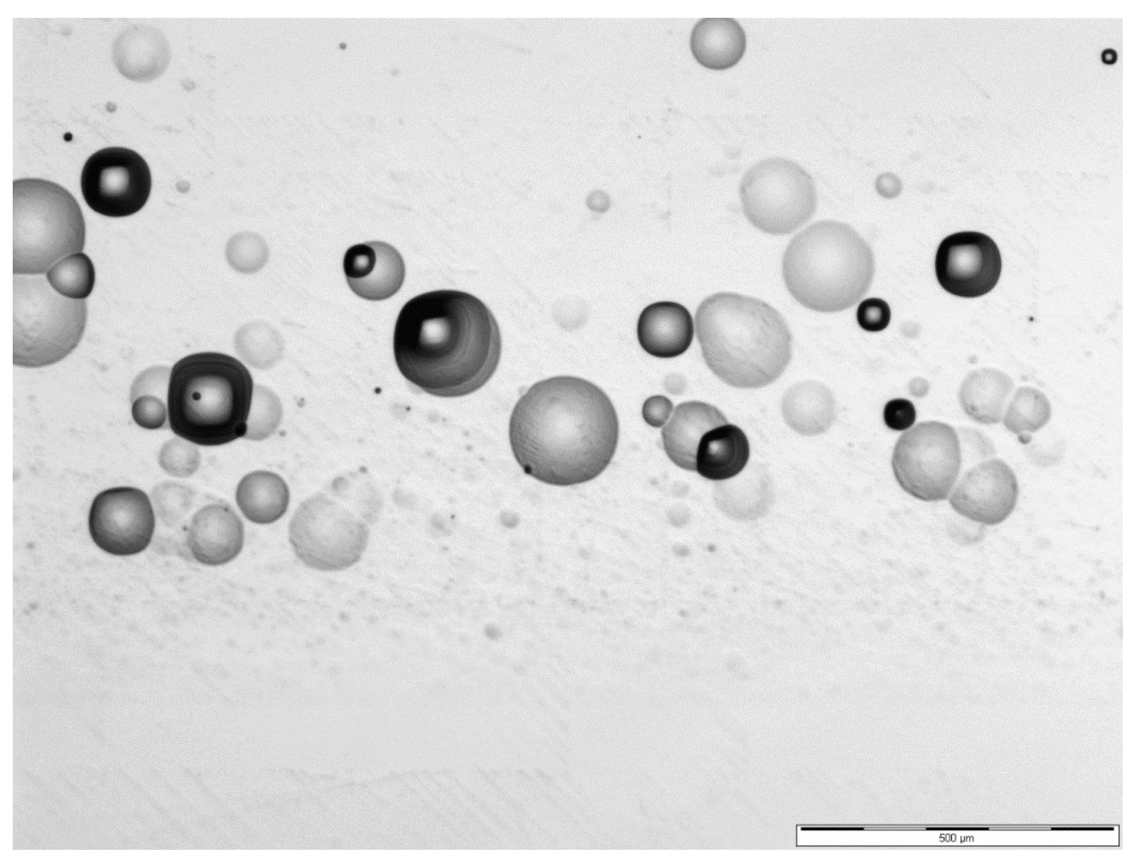


Instabilities at the phase boundary [2]

Constitutional supercooling at the phase boundary [3]

$$\frac{G_L}{V} \geq \frac{(1-k)\cdot C_l \cdot (-m)}{k \cdot D} \cdot k_{BPS}$$

G_L: Temperature gradient in the melt
V: Pulling velocity
k: Equilibrium distribution coefficient
k_{BPS}: effective distribution coefficient
m: Slope of liquids line
D: Diffusion constant of doping specimen
C_l: Concentration of doping specimen in the liquid



Etch pits of several defects

Distribution of **point defects** changes with doping concentration [4]

$$C_{crit} = \frac{V}{G_s} = 1{,}34 \ x \ 10^{-3} \ {cm^2}/{Kmin}$$

V: Pulling velocity
G_s: Axial temperature gradient in the solid

Experimental & characterization

Growth of highly Arsenic and Phosphor doped Si crystals:

- n = 5-10x10^{19} atoms/cm³ [specific resistivity ~ 1 mΩcm]
- Crystals diameters of 5"

Experimental parameters of interest:

Thermal gradient G & growth speed v at the phase boundary

- G/v criterion by Hurle, Tiller, Careuthers [3]
- v/G criterion by Voronkov [4]

Thermal distribution

- Thermal stress

Form of crystal cone

- Peaked or flat cone (regulation through pull speed and heater power)

Dopant element

- Covalent radii of varying dopant element cause different level of stress (compression or tension)

Characterization methods:

Problem: Most optical / non-destructive measurement methods do not succeed on highly doped silicon e.g. fourier transform infrared spectroscopy (FTIR), lateral photovoltage scanning (LPS)

Dislocations:

- Etch pits through chemical etching (Schimmel, Seiter)
- X-ray topography (XRT)

Oxygen content

- Gas Fusion Analysis (GFA)
- Secondary Ion Mass Spectroscopy (SIMS)

Dopant content

- Secondary Ion Mass Spectroscopy (SIMS)
- Resistivity measurements (4 point prober)

Lattice constant

- X-ray diffraction (XRD)

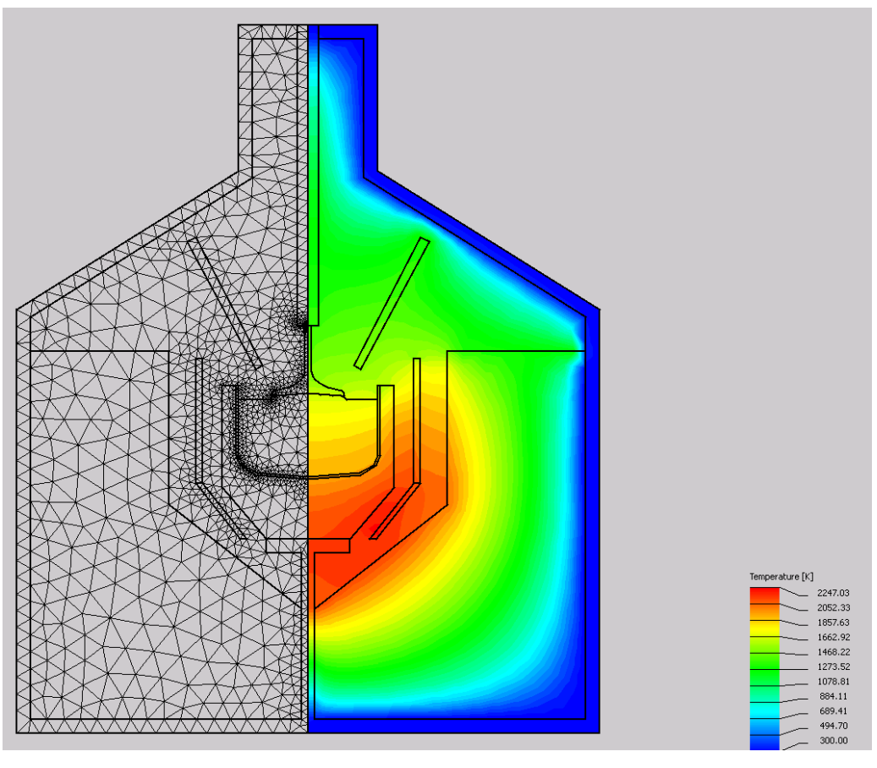
Point defects

- OSF ring distribution (oxidation + etching)

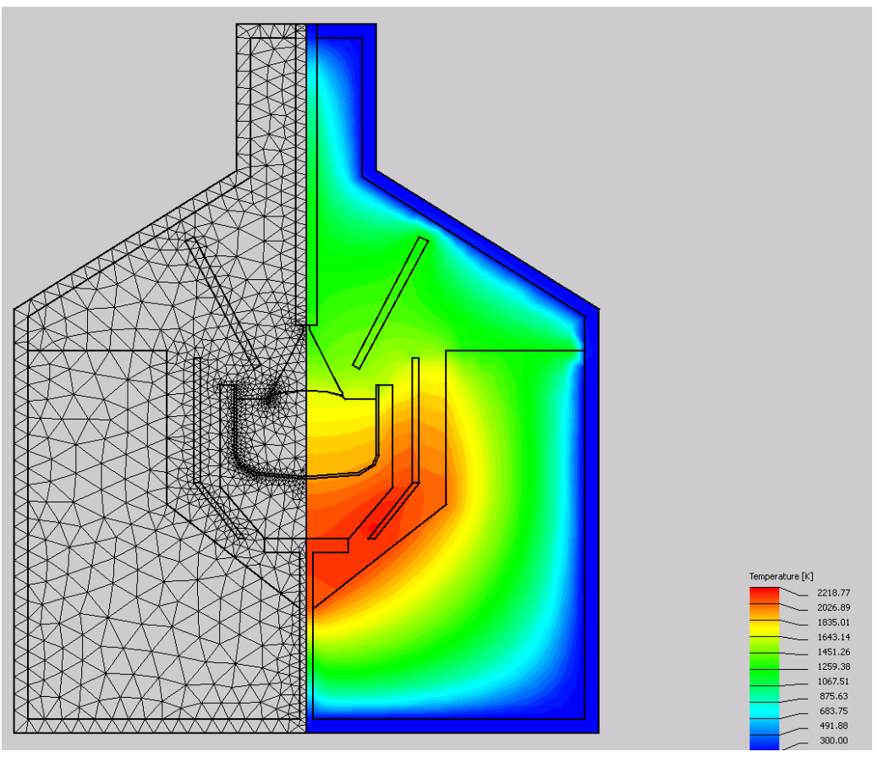
Phase boundary

- Photoluminescence (PL)
- Chemical etching

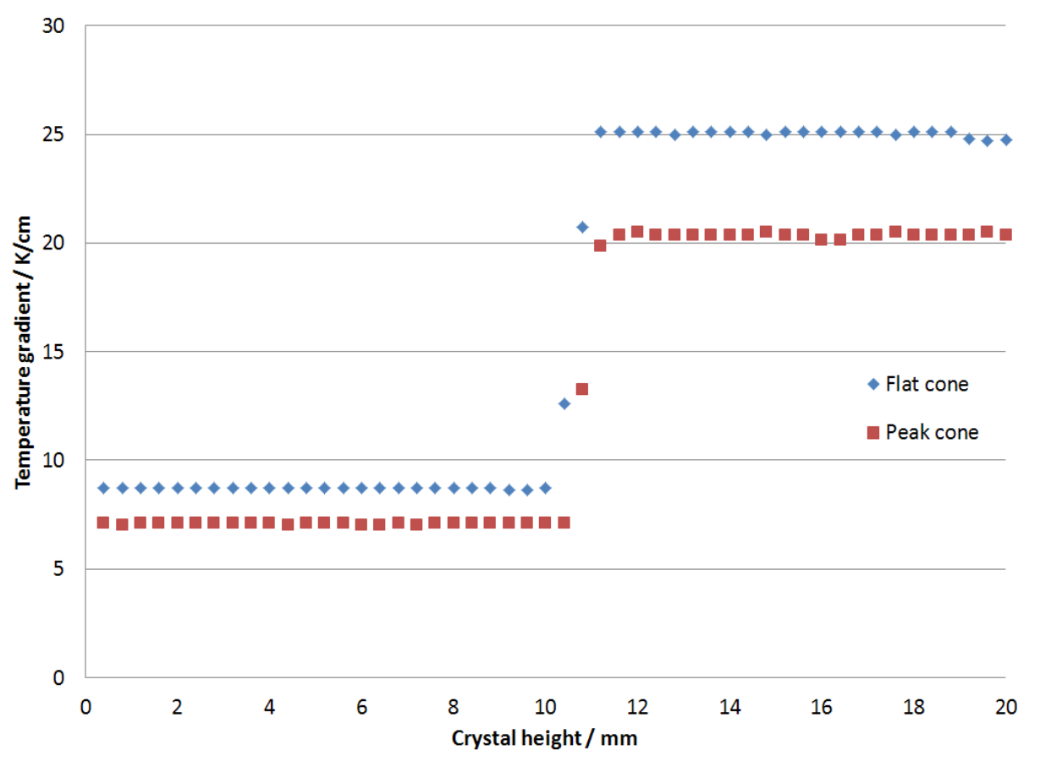
CrysMAS simulations



Flat cone



Peak cone



Temperature gradient G at the phase boundary

Simulations with CrysMAS of temperature distributions at the phase boundary for different crystal geometries to determine its influence on e.g. the thermal gradient G

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