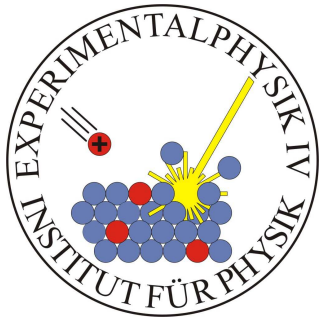


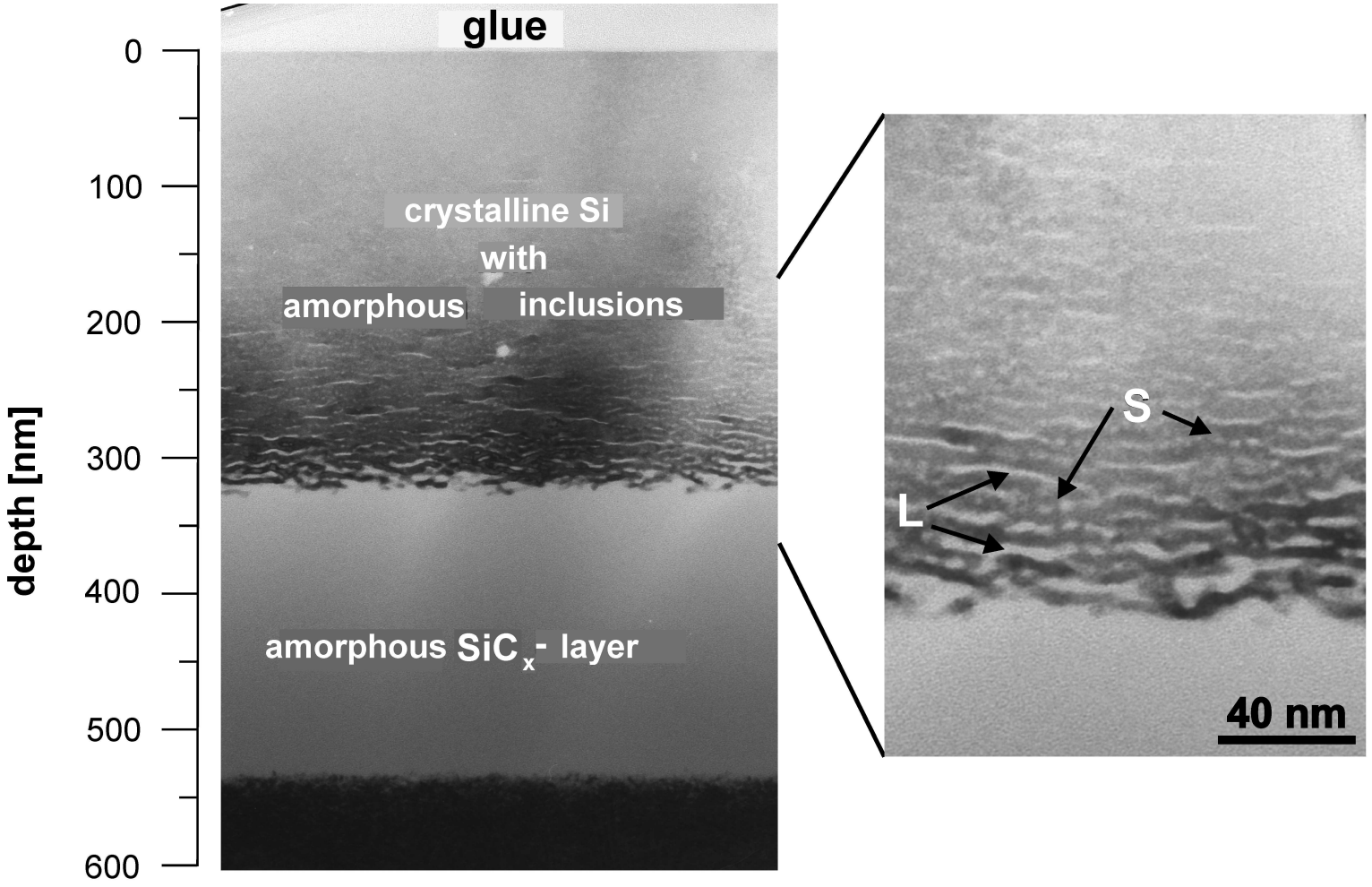
Monte Carlo simulation study of a selforganization process leading to ordered precipitate structures

F. Zirkelbach, M. Häberlen, J. K. N. Lindner und B. Stritzker

Outline

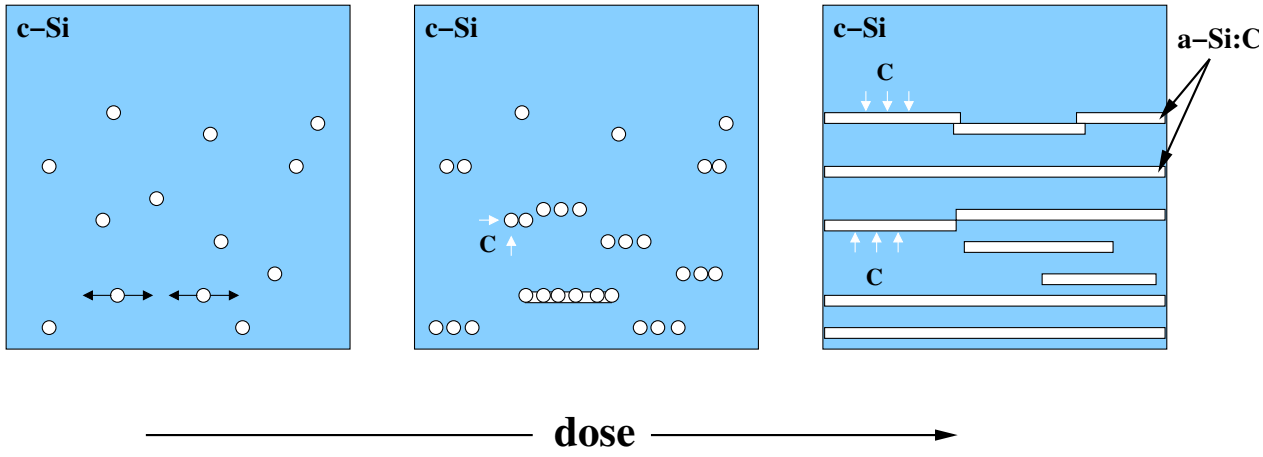
- Cross-section TEM: selforganized SiC_x-precipitates
- Model describing the selforganization process
- Monte Carlo simulation
- Comparison of experiment and simulation
- Recipe for thick films of ordered laemllae
- Summary

Cross-Section TEM image showing selforganized amorphous lamellar inclusions



$180keV\ C^+ \rightarrow Si(100)$, 150 °C, $4.3 \times 10^{17} cm^{-2}$

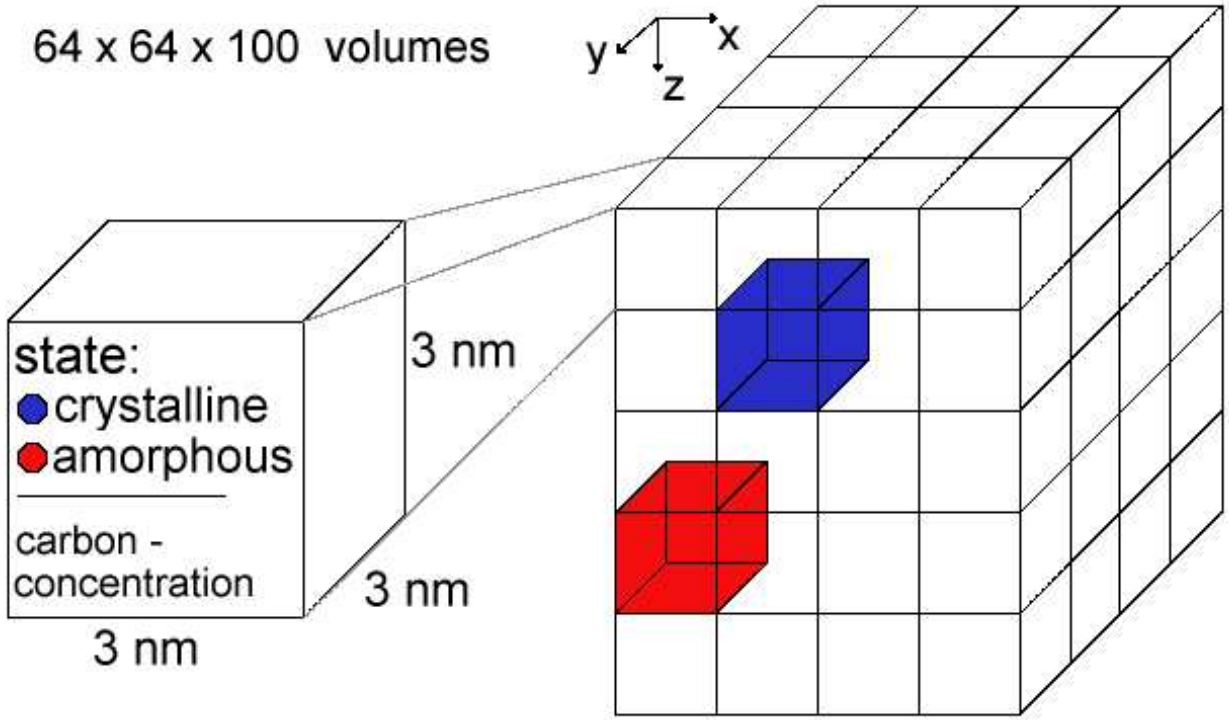
Model



- Supersaturation of C in $c-Si$
  $\rightarrow$ **Carbon induced** nucleation of spherical SiC_x-precipitates
- High interfacial energy between $3C-SiC$ and $c-Si$
  $\rightarrow$ **Amorphous** precipitates
- $20-30\,\%$ lower silicon density of $a-SiC_x$ compared to $c-Si$
  $\rightarrow$ **Lateral strain** (black arrows)
- Implantation range near surface
  $\rightarrow$ **Relaxation** of **vertical strain component**
- Reduction of the carbon supersaturation in $c-Si$
  $\rightarrow$ **Carbon diffusion** into amorphous volumina (white arrows)
- Remaining lateral strain
  $\rightarrow$ **Strain enhanced** lateral amorphization
- Absence of crystalline neighbours (structural information)
  $\rightarrow$ **Stabilization** of amorphous inclusions **against recrystallization**

Simulation

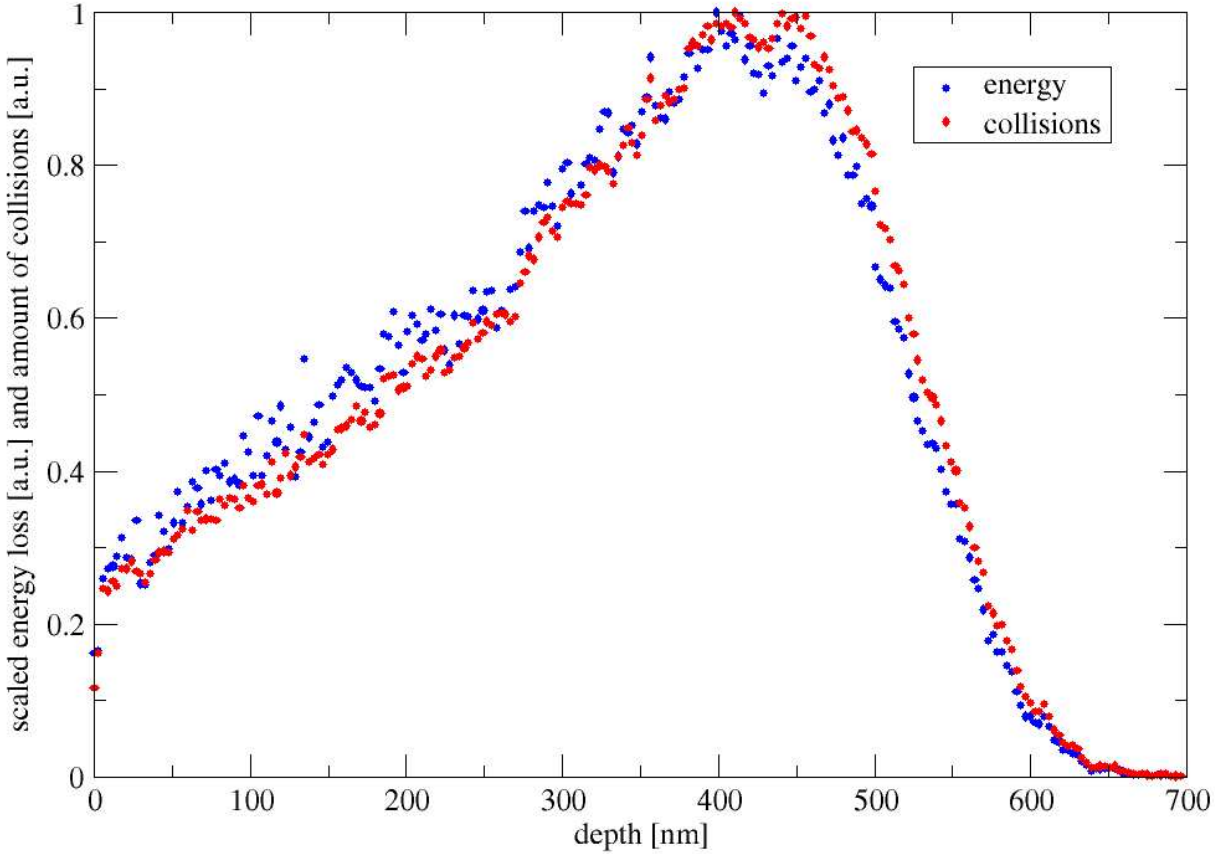
Discretization of the target



- divided into cells with a cube length of $3\,nm$
- periodic boundary conditions in x,y-direction

Simulation

TRIM collision statistics



- identical depth profiles for number of collisions per depth and nuclear stopping power
- mean constant energy loss per collision

Simulation algorithm

The simulation algorithm consists of the following three parts looped s times corresponding to a dose $D = s/(64 \times 64 \times (3\,nm)^2)$:

- Amorphization / Recrystallization
- Carbon incorporation
- Diffusion / Sputtering

Amorphization / Recrystallization

- random numbers distributed according to the nuclear energy loss
  → determine the volume in which a collision occurs
- compute local probability for amorphization / recyrstallization
- let another random number decide ...

$$p_{c\to a}(\vec{r}) = p_b \quad + \quad p_c\, c_{Carbon}(\vec{r}) \quad + \sum_{amorphous\, neighbours} \frac{p_s\, c_{Carbon}(\vec{r'})}{(\vec{r}-\vec{r'})^2}$$

normal (ballistic) **carbon inuced** **stress enhanced**

$$p_{a\to c}(\vec{r}) = (1 - p_{c\to a}(\vec{r}))\left(1 - \frac{\sum_{direct\, neighbours} \delta(\vec{r'})}{6}\right),$$

$$\delta(\vec{r}) = \begin{cases} 1 & \text{if volume } \vec{r} \text{ is amorphous} \\ 0 & \text{else} \end{cases}$$

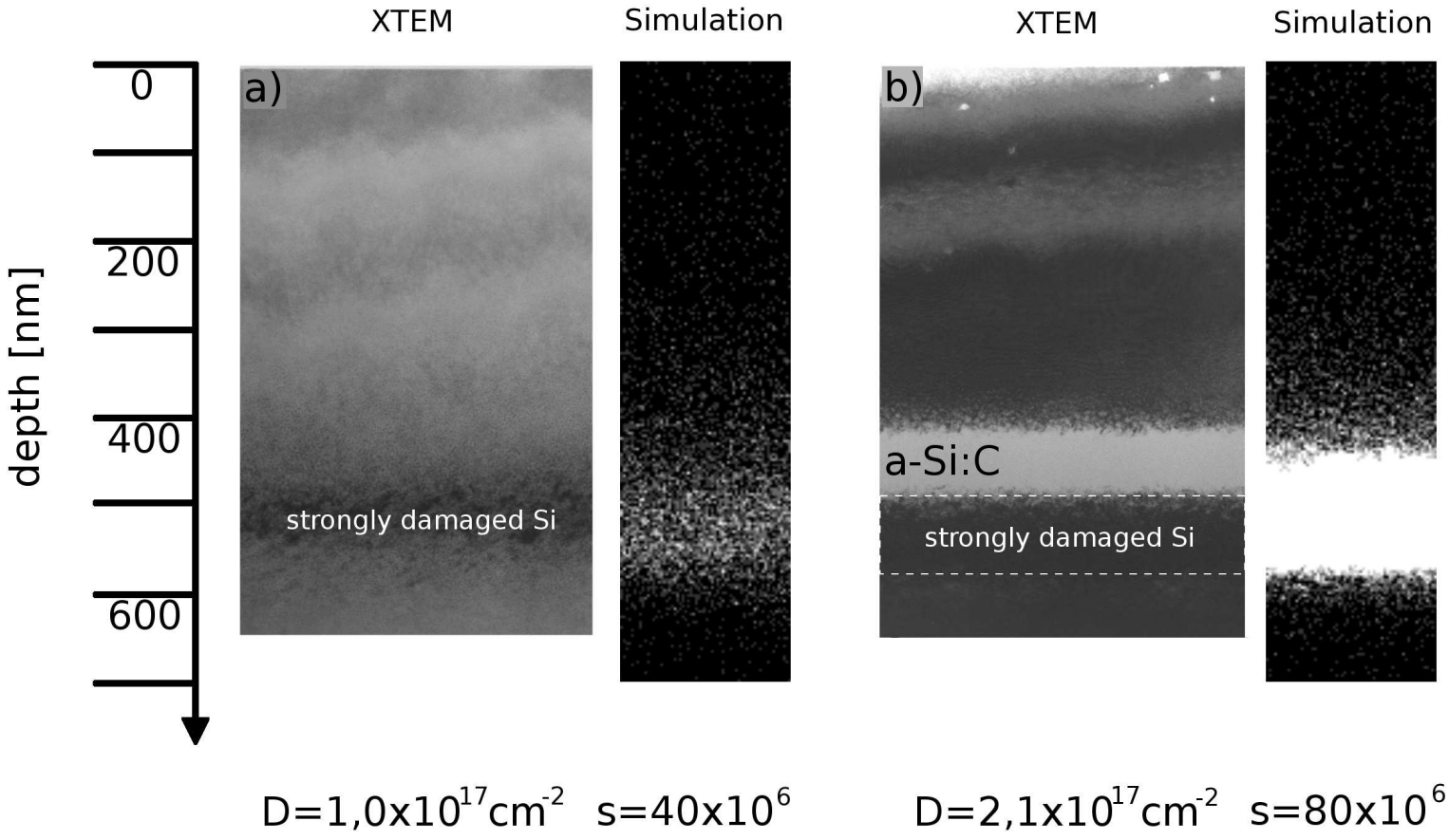
Carbon incorporation

- random numbers distributed according to the implantation profile to determine the incorporation volume
- increase the amount of carbon atoms in that volume

Diffusion/Sputtering

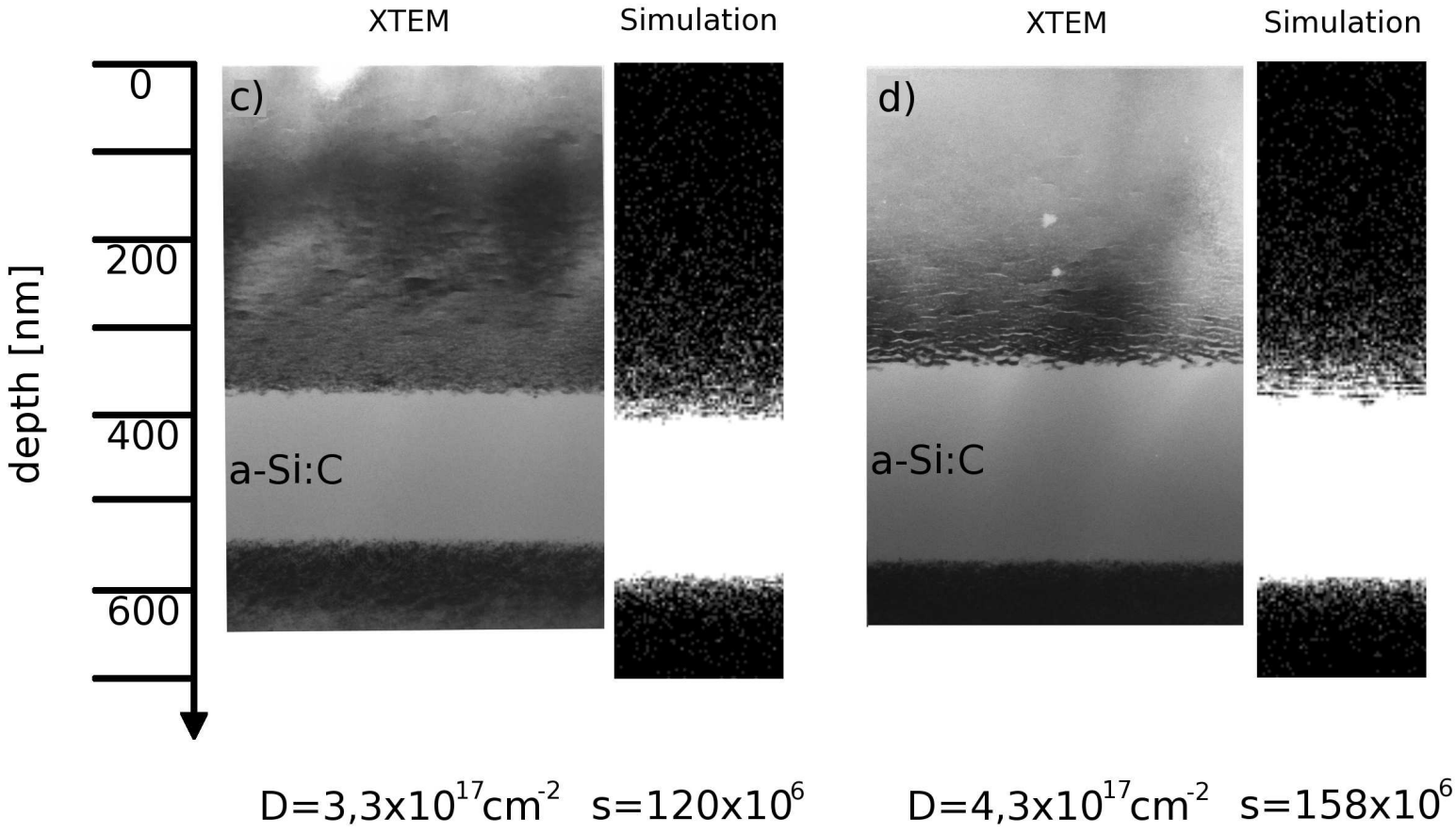
- every d_v steps transfer of a fraction d_r of carbon atoms from crystalline volumina to an amorphous neighbour volume
- remove $3\,nm$ surface layer after n loops, shift remaining cells $3\,nm$ up and insert an empty, crystalline $3\,nm$ bottom layer

Comparison of experiment and simulation



Simulation parameters:
$p_b = 0.01$, $p_c = 0.001 \times (3\,nm)^3$, $p_s = 0.0001 \times (3\,nm)^5$, $d_r = 0.05$, $d_v = 1 \times 10^6$.

Comparison of experiment and simulation



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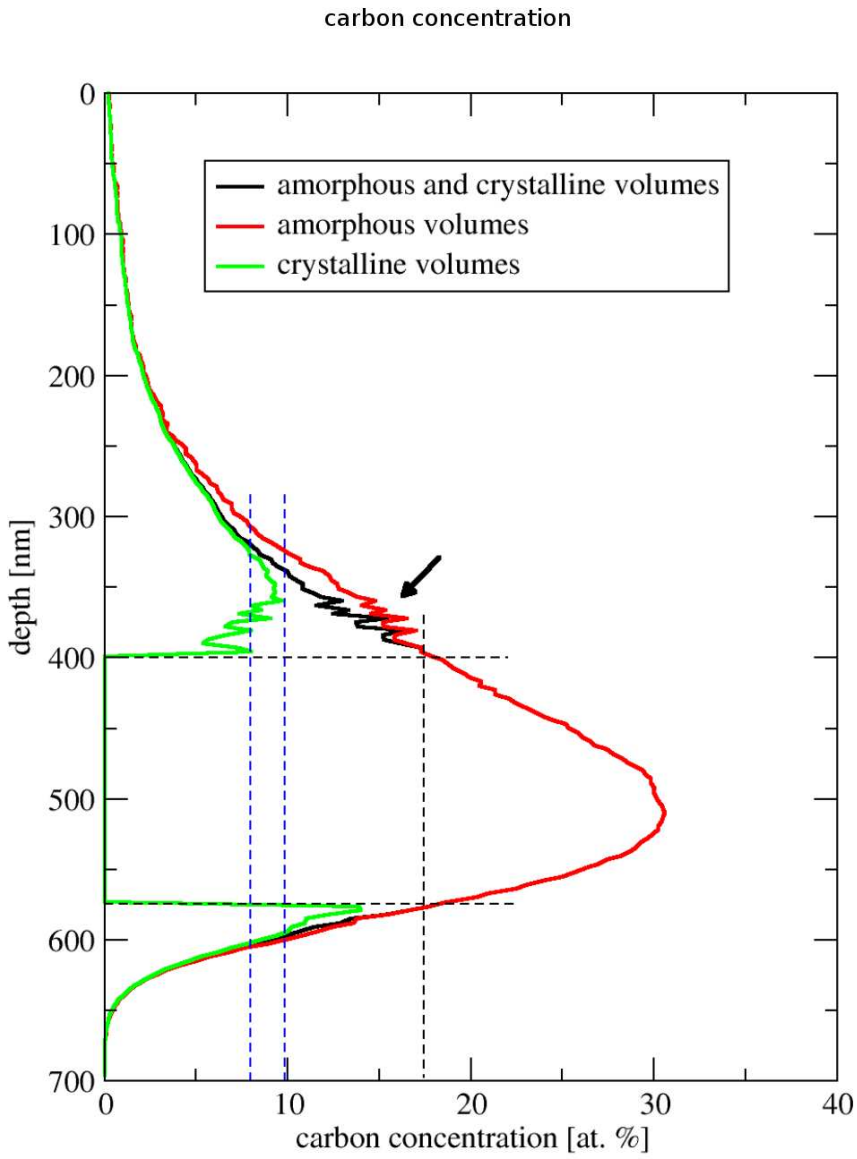
Conclusion:

- Simulation in good agreement with experimentally observed formation and growth of the continuous amorphous layer
- Lamellar precipitates and their evolution at the upper a/c interface with increasing dose is reproduced

Simulation is able to model the whole depth region affected by the irradiation process

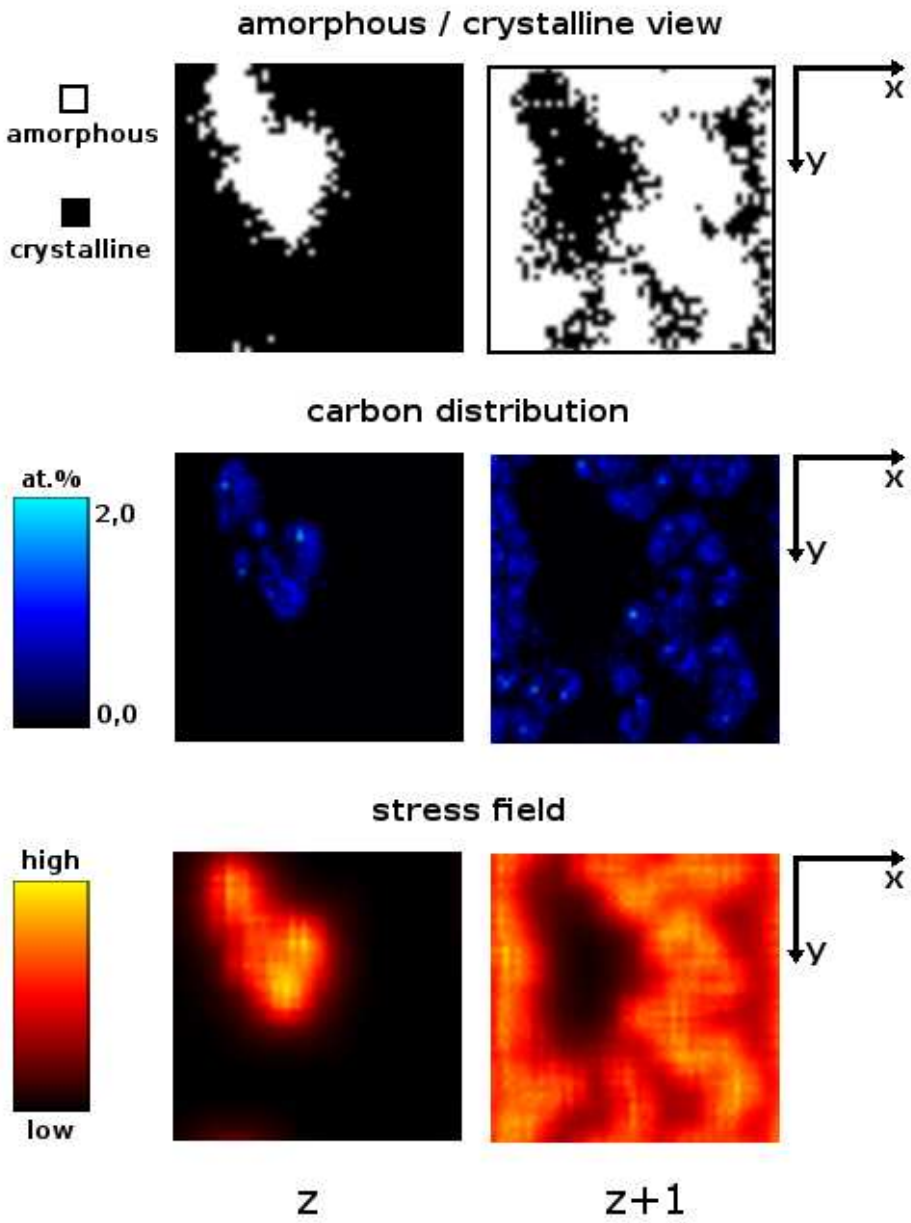
Structural/compositional information

- Fluctuation of the carbon concentration in the region of the lamellae
- Saturation limit of carbon in c-Si under given implantation conditions between 8 and 10 $at.\%$



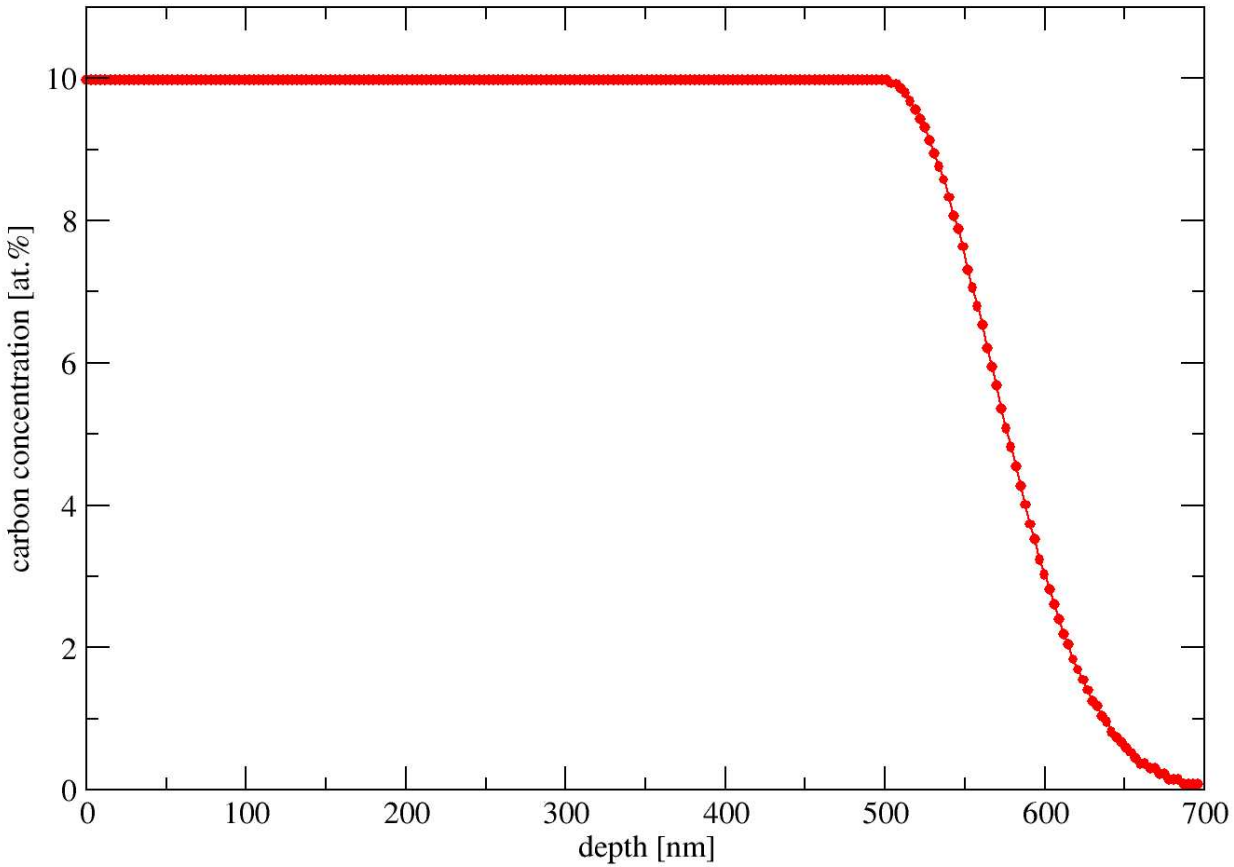
Structural/compositional information

- Complementarily arranged and alternating sequence of layers with high and low amount of amorphous regions
- Carbon accumulation in the amorphous phase



Recipe for thick films of ordered lamellae

Prerequisites:
Crystalline silicon target with a nearly constant carbon concentration at $10\,at.\%$ in a $500\,nm$ thick surface layer

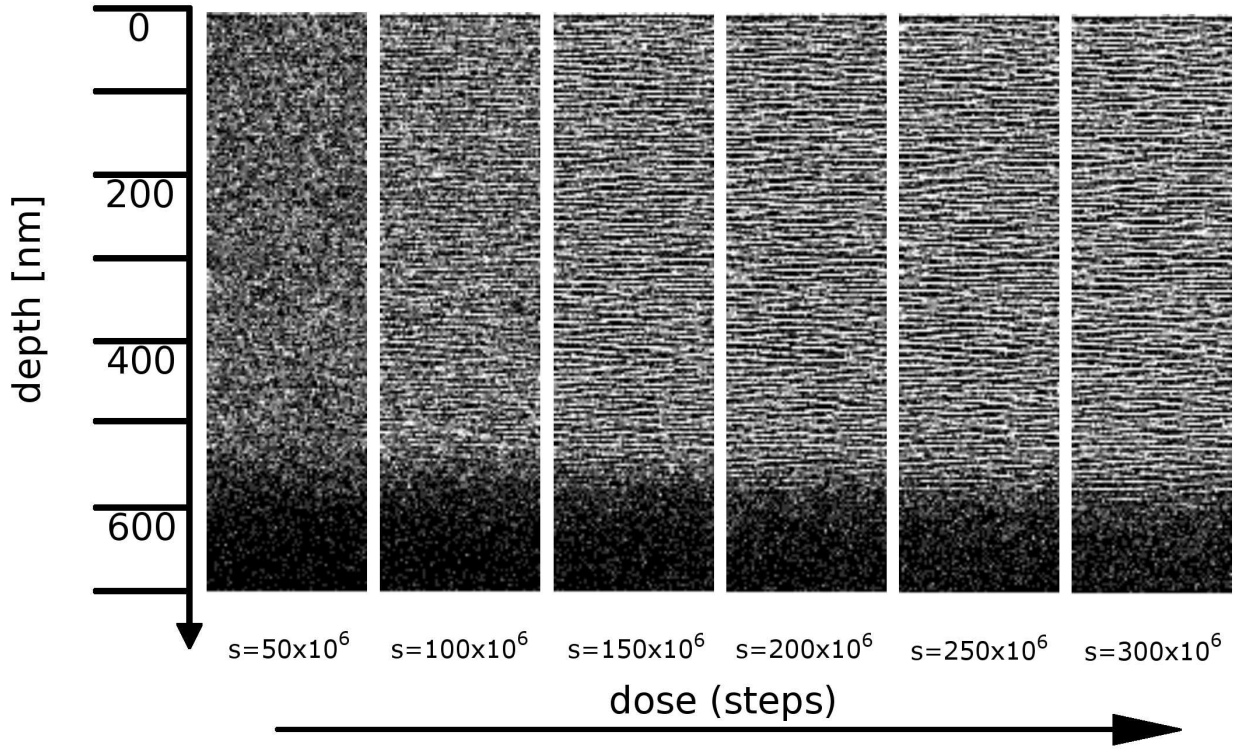


- Multiple energy (180-10 keV) $C^+ \rightarrow Si$ implantation
- $T_i = 500\,^\circ\mathrm{C}$, to prevent amorphization

Recipe for thick films of ordered lamellae

Stirring up: $2\,MeV\ C^+ \rightarrow Si$ irradiation step at 150 °C

- This does not significantly change the carbon concentration in the top $500\,nm$
- Nearly constant nuclear energy loss in the top $700\,nm$ region



Starting point for materials showing strong photoluminescence

Dihu Chen et al. Opt. Mater. 23 (2003) 65.

Summary

- Observation of selforganized nanometric precipitates by ion irradiation
  $C \rightarrow Si \qquad T_i : 150 - 350\,^{\circ}\mathrm{C} \qquad D \leq 8 \times 10^{17} cm^{-2}$
- Model proposed describing the selforganization process
- Model implemented in a Monte Carlo simulation code
- Modelling of the complete depth region affected by the irradiation process
- Simulation is able to reproduce entire amorphous phase formation
- Precipitation process gets traceable by simulation
- Detailed structural/compositional information available by simulation
- Recipe proposed for the formation of thick films of lamellar structure

Thank you for your attention!
Thanks for accepting me as a guest!

. . . another recipe I propose:

- 06 cl vodka
- 03 cl peach liqueur
- 03 cl amaretto
- 16 cl black currant juice
- dash of citron
- 3-4 ice cubes

$\Rightarrow$ Killer Cool Aid