Monte Carlo Study of Stacking Fault Interactions during 3C-SiC Epitaxial Growth

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3C-SiC has emerged as an attractive wide bandgap semiconducting material for high temperature, high frequency, and high voltage applications. It exhibits a low density of states at the 3C-SiC/SiO_2 interface, making it a viable material for power-switching MOSFETs which are of particular interest to motor drives in electric vehicles. Moreover, 3C-SiC can be grown on a Si substrate to drive down production costs. However, as a result of the 19.7% lattice mismatch between Si and 3C-SiC, a high density of stacking faults are generated and a specific interaction between adjoining stacking faults generates an electrically active defect which can degrade the performance of 3C-SiC devices. Here we employ Monte Carlo simulations to better understand the interaction of stacking faults during epitaxial growth of 3C-SiC on a Si substrate. By modeling the generation, annihilation, and termination of stacking faults in 3C-SiC grown on the Si(100) face as well as the Si(111) face, we can compare the densities of stacking faults and electrically active defects for both geometries. For both cases, we monitored the evolution of defect density as a function of 3C-SiC film thickness for various different sizes of crystals ranging from 15×15 μm^2 to 1000×1000 μm^2. In contrast to that of (100)-oriented 3C-SiC, the stacking faults on the (111) face have unified polarities which gives rise to increased annihilation. Therefore, we expect to see that the stacking fault density will decrease more rapidly in the case of (111)-oriented 3C-SiC growth.

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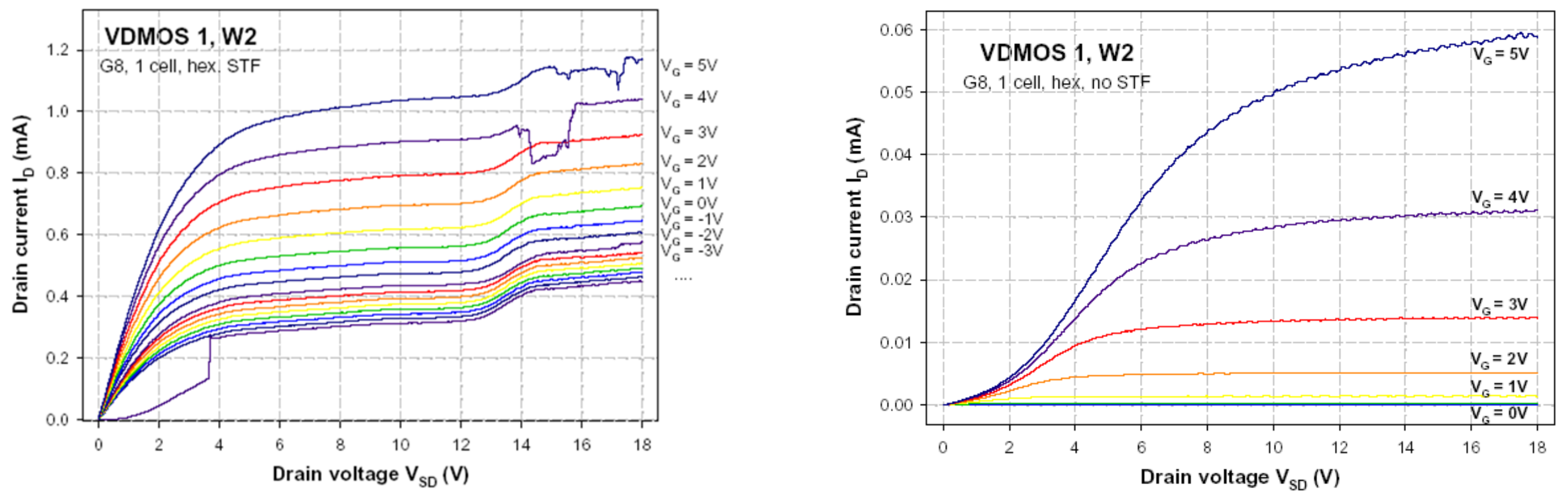
Motivation

3C-SiC shows promise for use in high temperature, high voltage, and high frequency power switching devices. However, large stacking fault densities within the crystal can degrade electrical properties. Therefore, it is important to study stacking fault interactions during epitaxial growth so that defect reduction can be optimized.



High SF Density Low SF Density (<6000 cm^2)

Figure 1: Plots of drain current versus drain voltage for power MOSFETs synthesized from 3C-SiC[1]

Goal: Monitor stacking fault density reduction during epitaxial growth for various crystal sizes and orientations

Stacking Faults (SFs) in 3C-SiC

- SFs are generated at the interface between the 3C-SiC crystal and Si substrate during epitaxial growth in order to minimize the incoherence generated by the 19.7% lattice mismatch
- SFs propagate along the four equivalent {111} planes of 3C-SiC

3C-SiC(001) Face

4 Orientations of SFs expressed:

- 2 with Carbon Polarity
- 2 with Silicon Polarity
- **C polar and Si polar SFs are related by 90º rotations**

3C-SiC(111) Face

3 Orientations of SFs expressed:

- All have unified polarity
- Propagate along (11-1), (1-11), and (-111)

SF Interactions:

SFs with like polarity: one will annihilate the other

SFs with distinct polarity: each terminate the other's propagation

Point defects at SF junctions can introduce states into the band gap

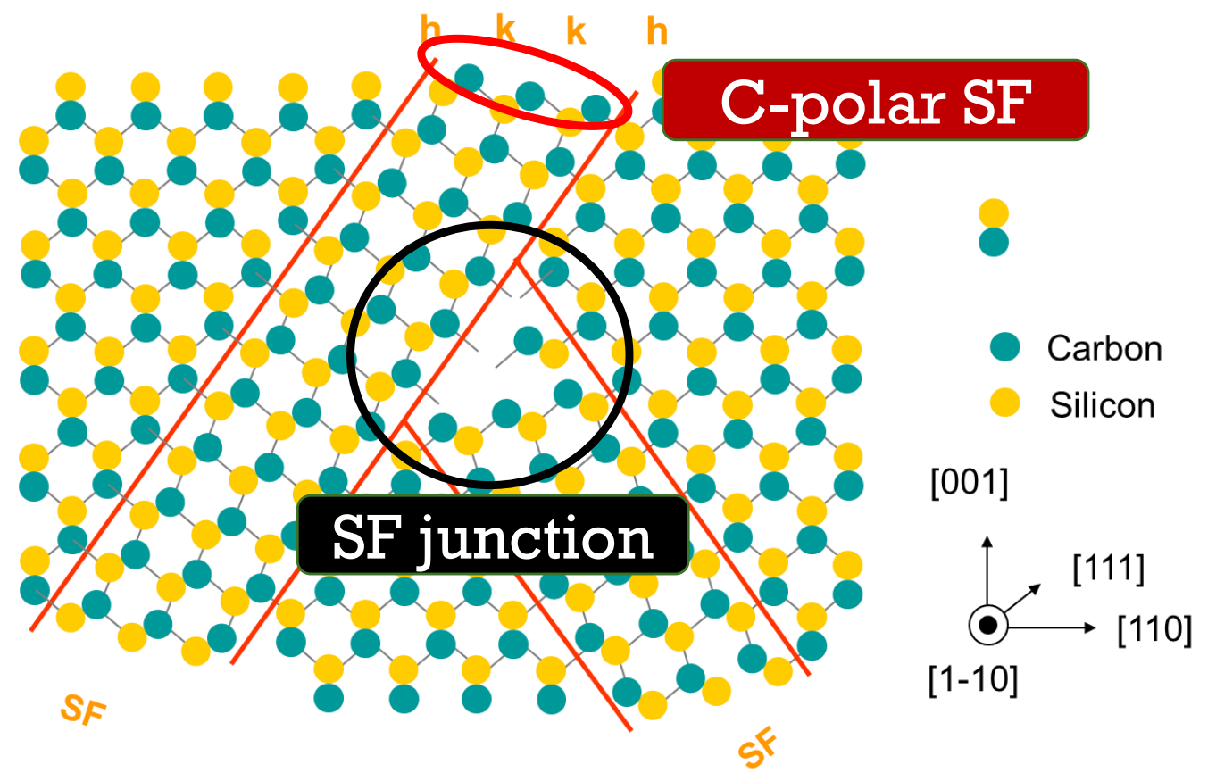


Figure 2. Diagram of intersecting stacking faults in 3C-SiC(001)

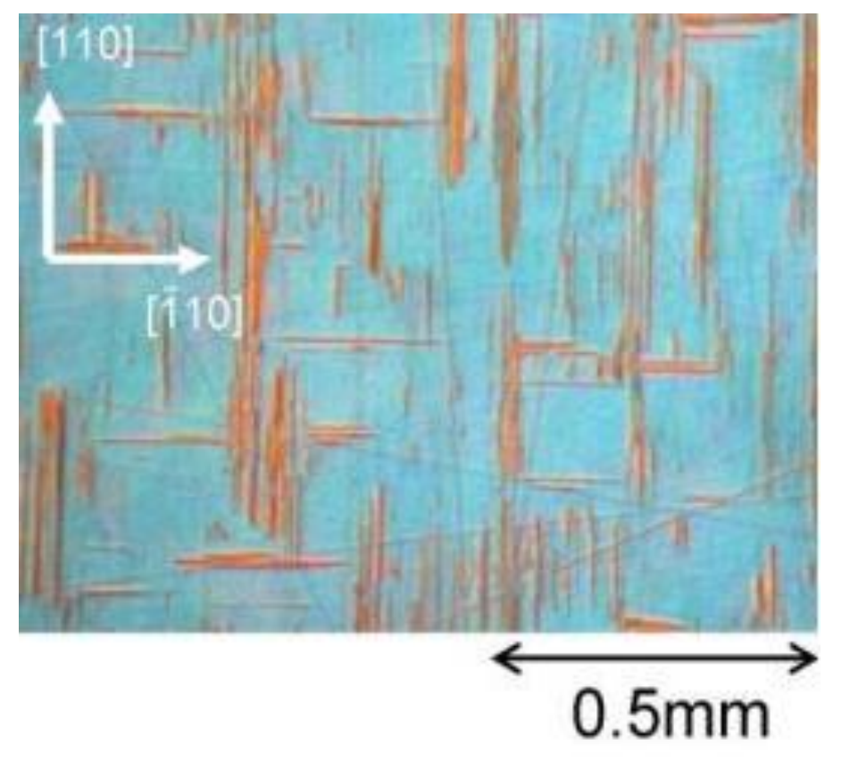
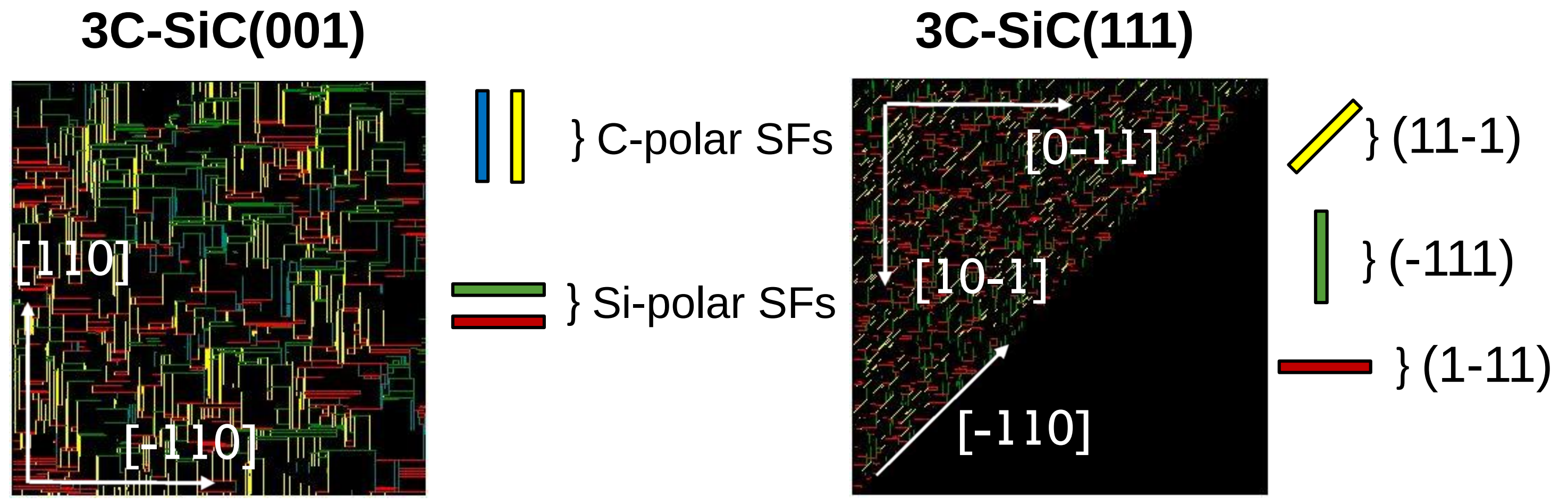


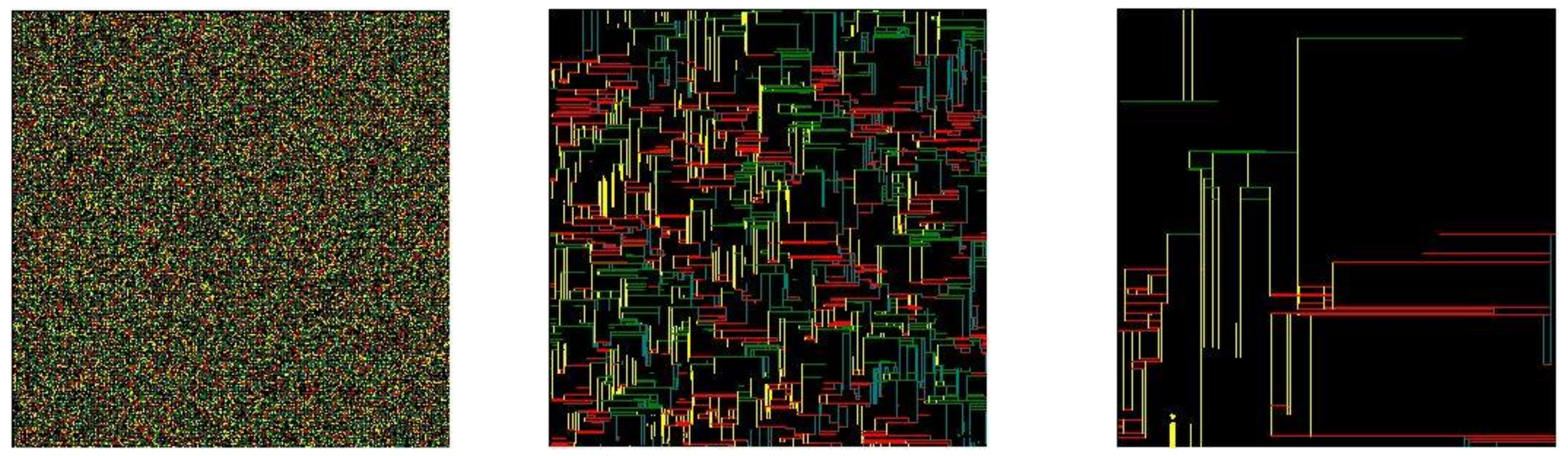
Figure 3. 3C-SiC surface after KOH etching to accentuate SFs[3]

Monte Carlo Simulation

Geometry of Simulation Setup:



Evolution of a SF Interaction Simulation:

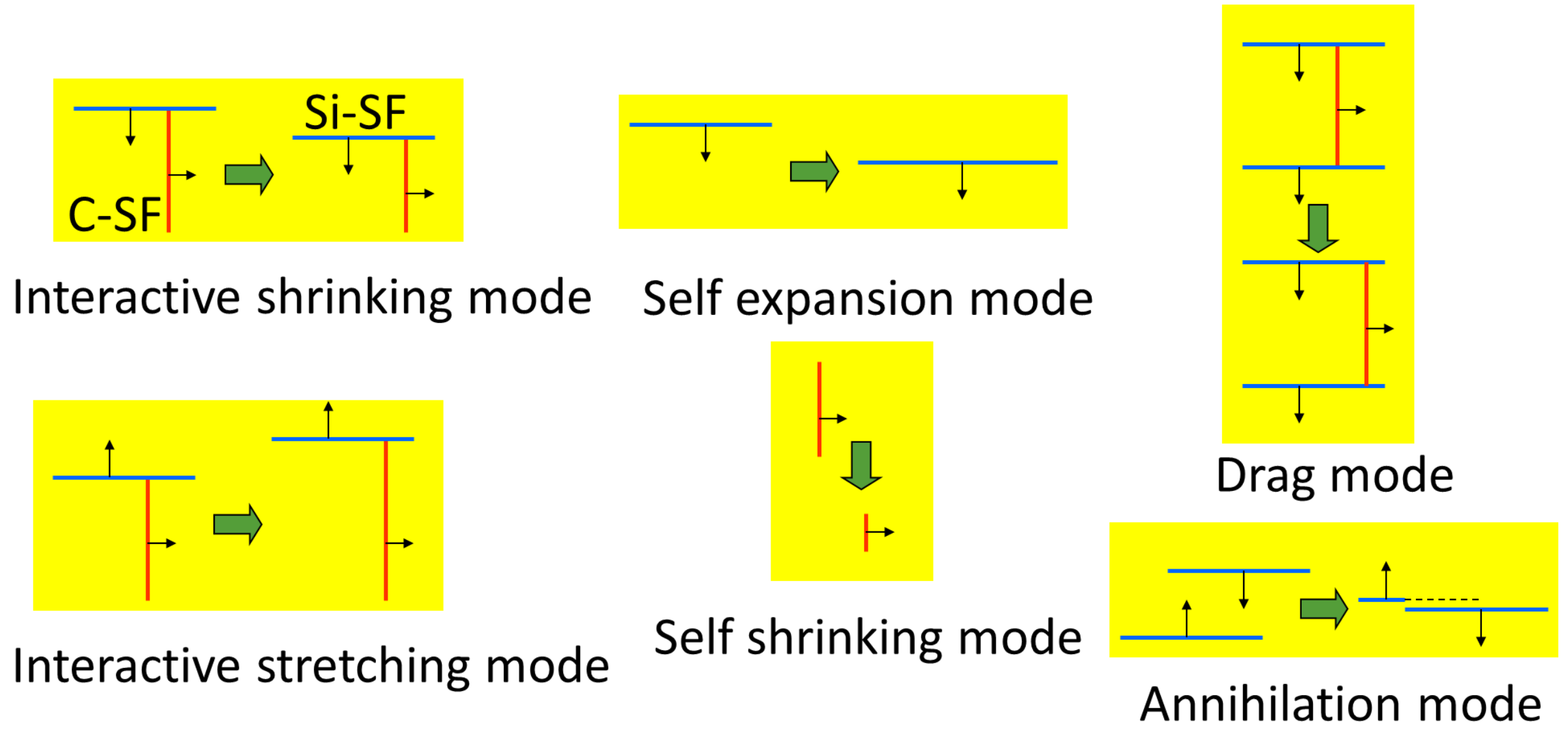


Initial Carbonization

SiC Thickness = 0.872 µm
SF Density = 2.4x10^5/cm

SiC Thickness = 5.232 µm
SF Density = 4.57x10^4/cm

Summary of Stacking Fault Interactions[4]:



Interactive shrinking mode

Self expansion mode

Drag mode

Interactive stretching mode

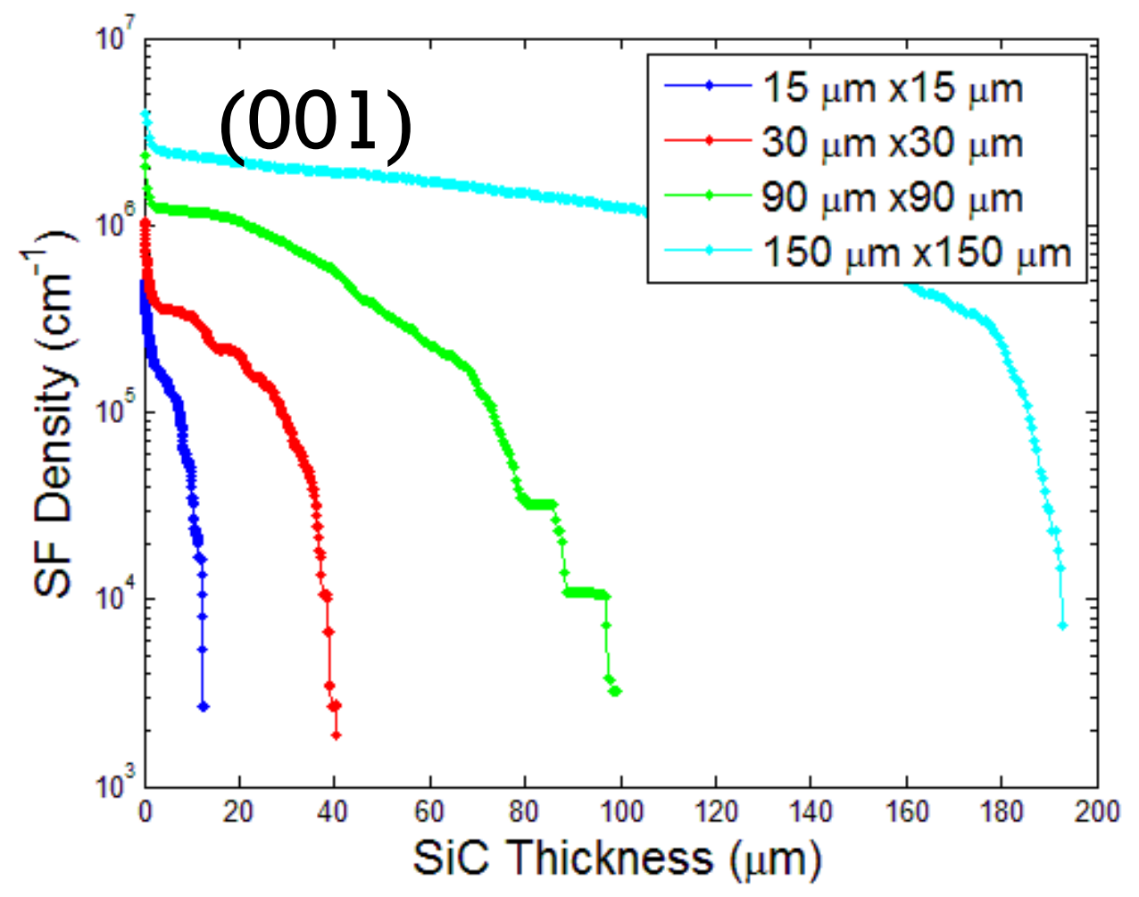
Self shrinking mode

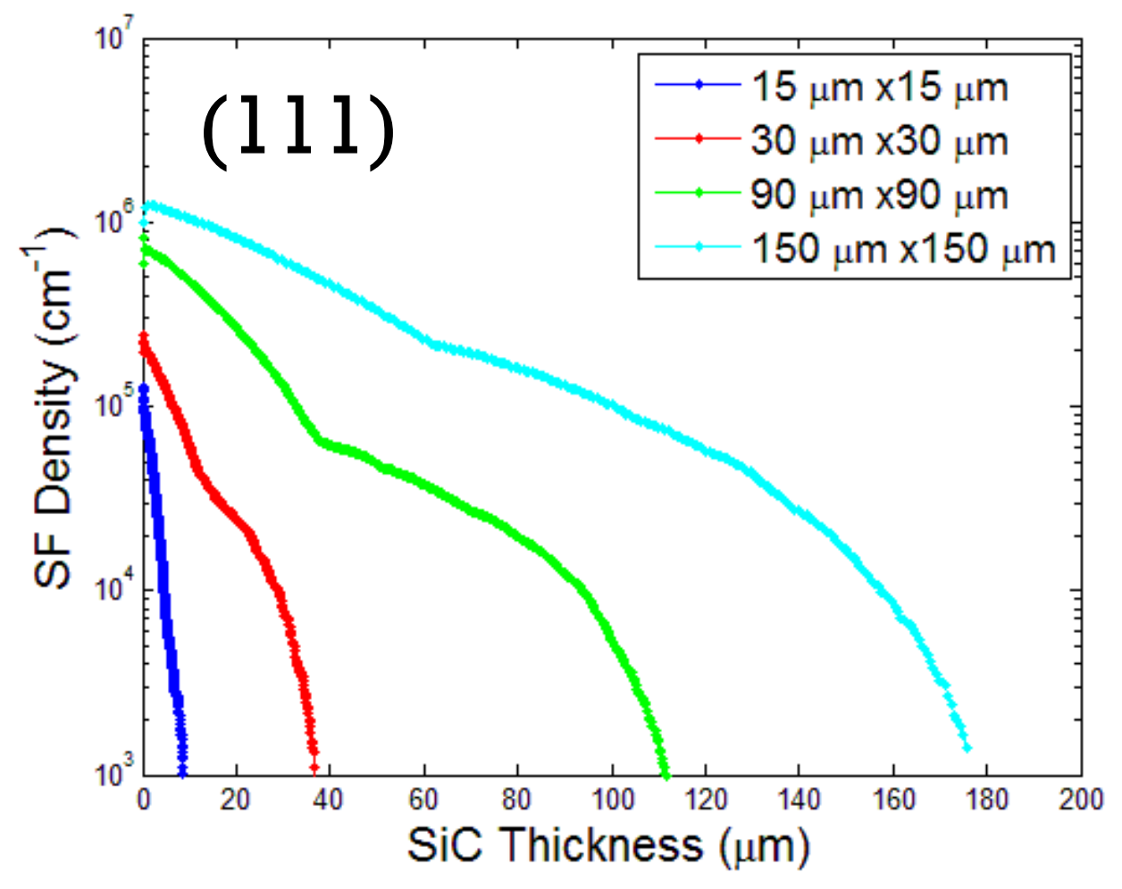
Annihilation mode

Key Simulation Parameters:

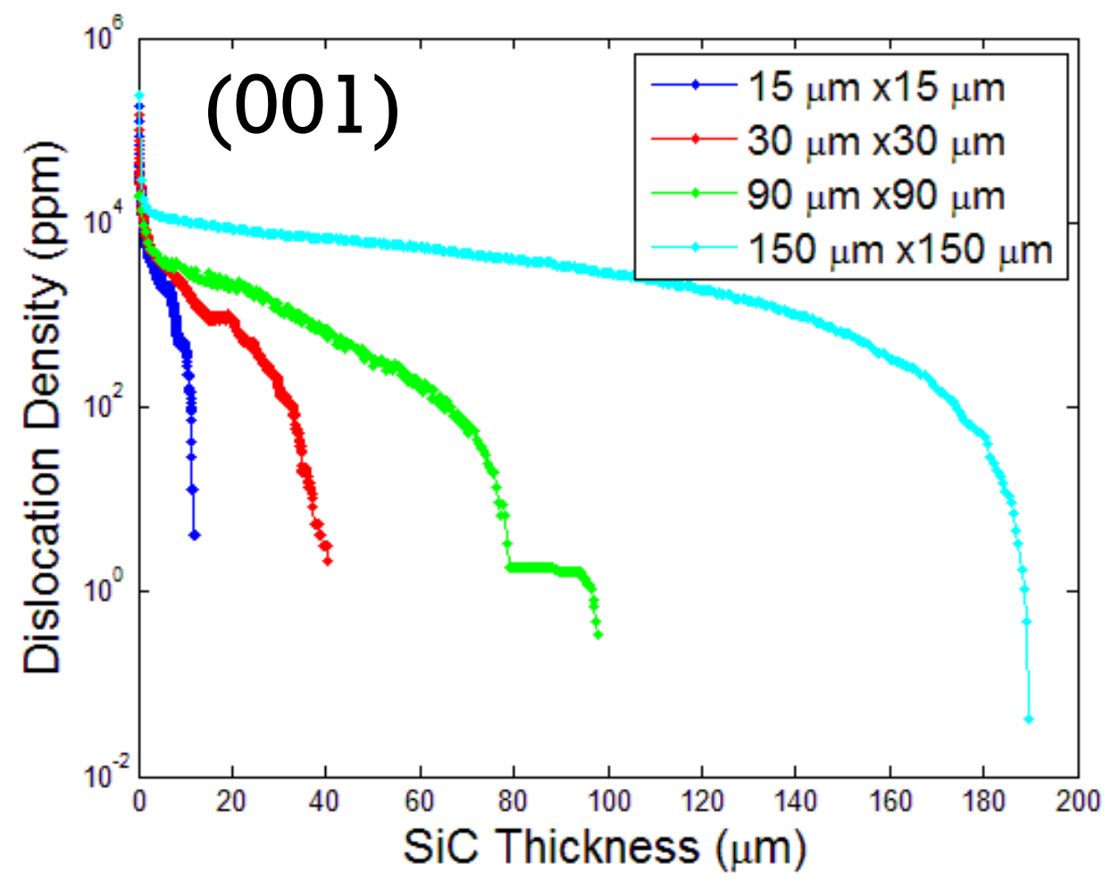
Static Generation Probability for SFs	12.5%	Expansion Probability	12.5% (for Si-polar SFs)
Annihilation Balance	50/50	Angle Offset	.125°

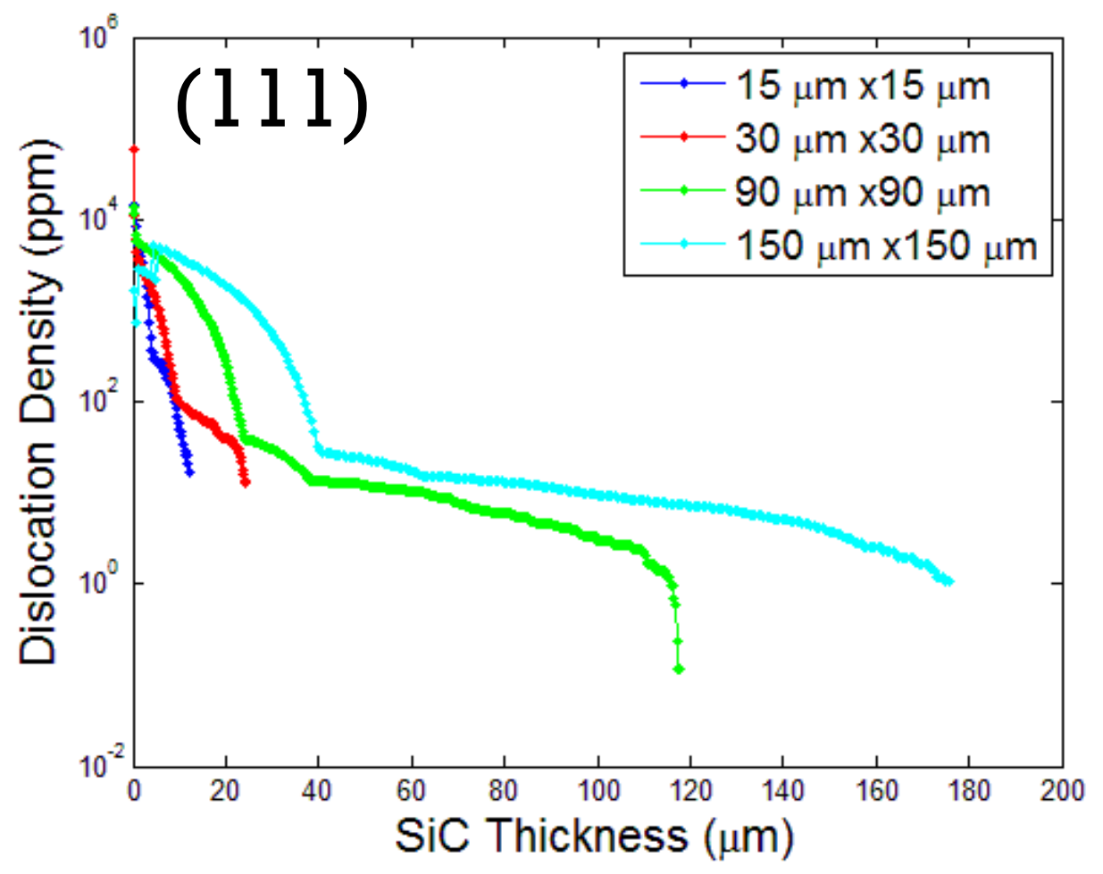
Stacking Fault Density Reduction



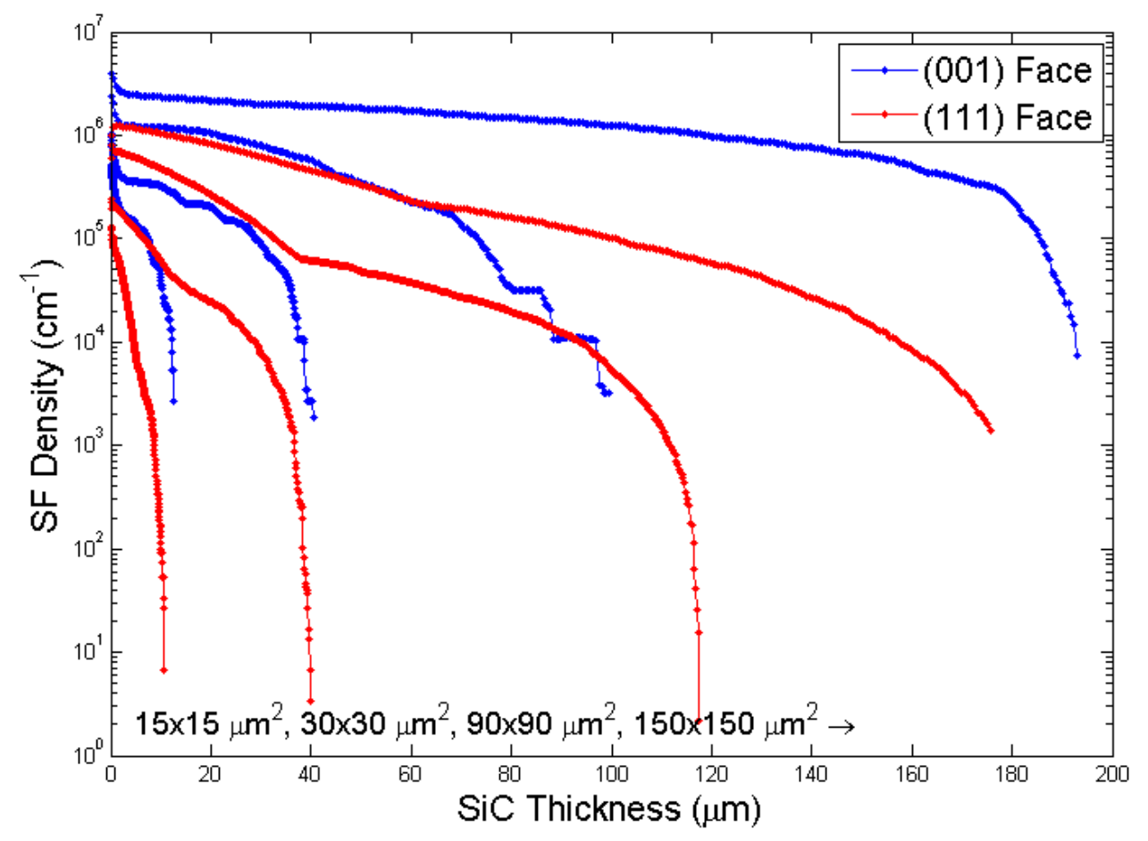


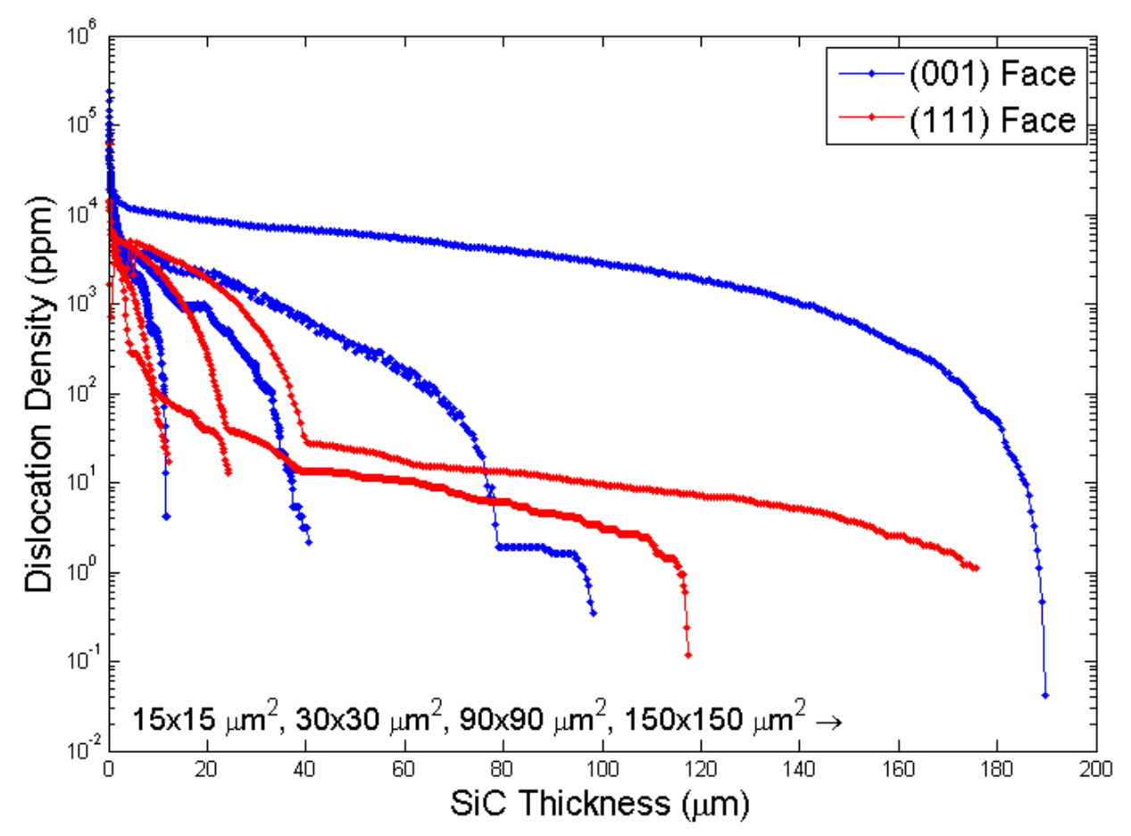
Dislocation (SF Edge) Density Reduction





Comparison between (001) and (111) Face





Conclusion

- SF density decreases with increasing thickness and decreasing crystal area size on both the 3C-SiC(001) and the 3C-SiC(111) surfaces as a result of annihilation and termination interactions
- At some specific thickness, determined by area size, stacking fault density decreases dramatically
- Stacking fault density decreases more rapidly on the (111) face than the (001) face

Future Work

Depending on the polarity, SFs in 3C-SiC may be terminated by Shockley-type partial dislocations which can glide and interact along the four equivalent {111} planes. The glide of dislocations can change the dimensions of the stacking fault.

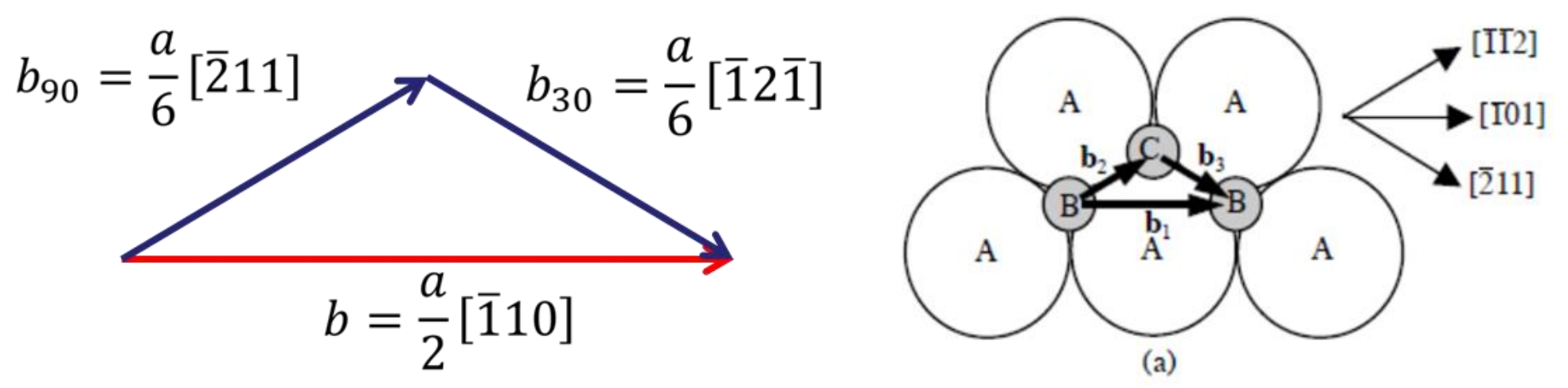
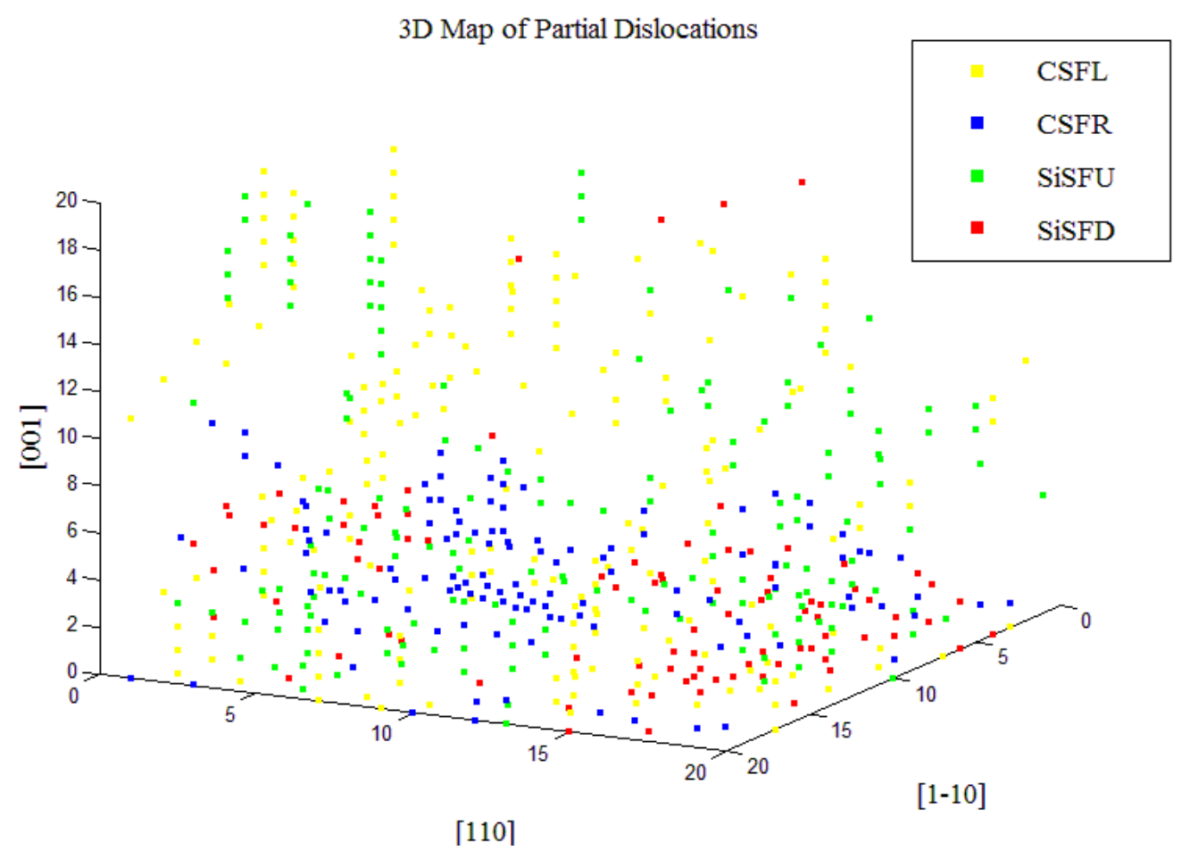


Figure 4. SFs are bordered by 30º and 90º partial dislocations which glide parallel to their Burger's vectors[5]



Future simulations can be made more comprehensive by employing 3D mapping of partial dislocations and incorporating dislocation glide into the algorithm.

Figure 5. 3D map of dislocations during simulation on 3C-SiC(001)

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