3D Simulations of Interacting Gliding Dislocation in 3C-SiC(001)

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3C-SiC has been identified as a leading semiconducting material for use in high, voltage, temperature, and frequency devices. In contrast to the other SiC polytypes, 3C-SiC has shown great potential through its high saturated electron drift velocity. The material also shows a very low density of states at the 3C-SiC/ SiO_2 interface making it an attractive option for use in power-switching MOSFETs. However, stacking faults form due to the 19.7% lattice mismatch at the 3C-SiC/ SiO_2 interface, and then expand throughout epitaxial growth, eventually terminating with other stacking faults, creating electrically active defects that lead to the electrical degradation of the material. After the epitaxial growth process has finished, the gliding of the partial dislocations at the edges of the stacking faults, instigated by the intrinsic shear stress of the system, begin to generate forest dislocations. The forest dislocations are created by the intersection of the counter pair of carbon-terminated stacking faults along the (-111) and (1-11) planes and the silicon-terminated stacking faults along the (111) and (-1-11) planes. By employing Monte Carlo simulations to model the generation of the dislocations we are able to analyze the density of forest dislocations throughout the system as a function of the shear stress, as well as a function of the temperature, material thickness, and stacking fault density. The results will allow for greater insight into the mechanisms by which leakage current density increases and how the generation of electrically active defects can be reduced through more sophisticated fabrication processes of 3C-SiC.

Interactions Between Gliding Dislocations in 3C-SiC (001)

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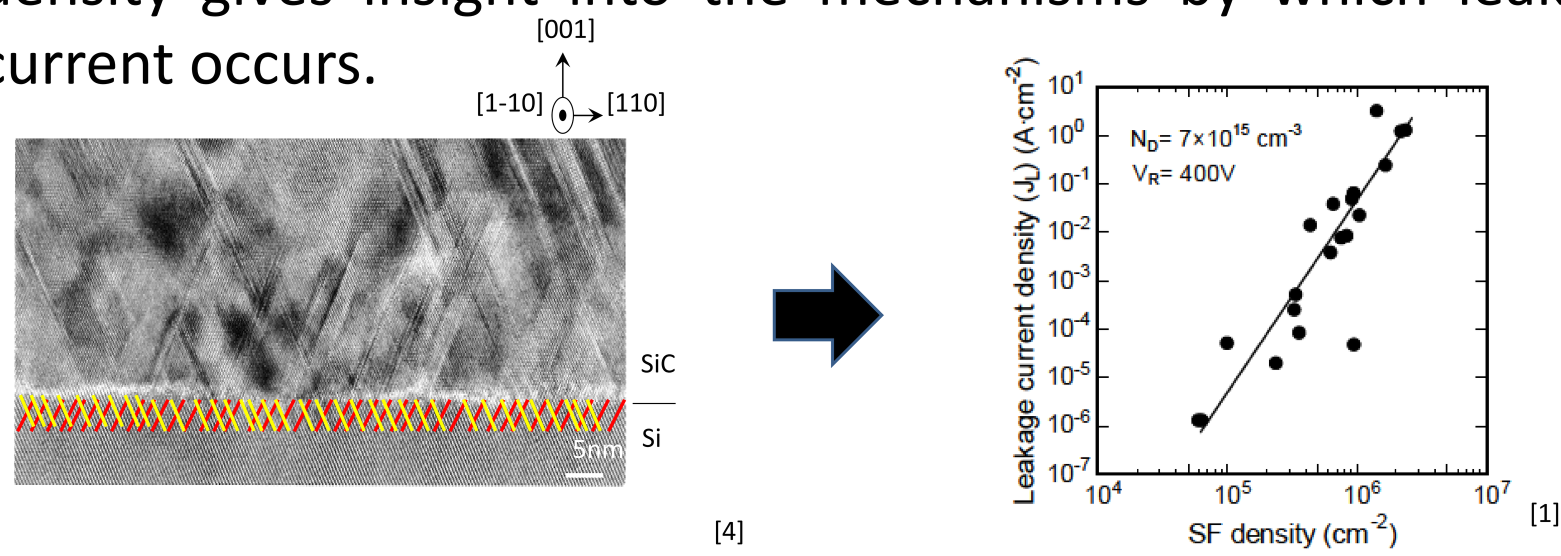
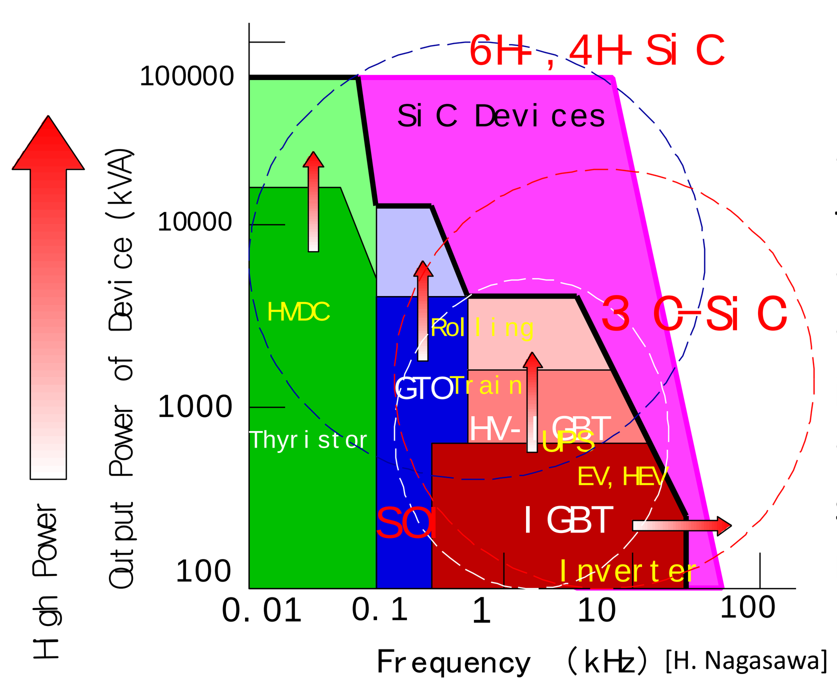
Motivation

3C-SiC is an attractive semiconducting material for use in a variety of high power electronic devices. The relationship between the forest dislocation (FD) and stacking fault (SF) density gives insight into the mechanisms by which leakage current occurs.



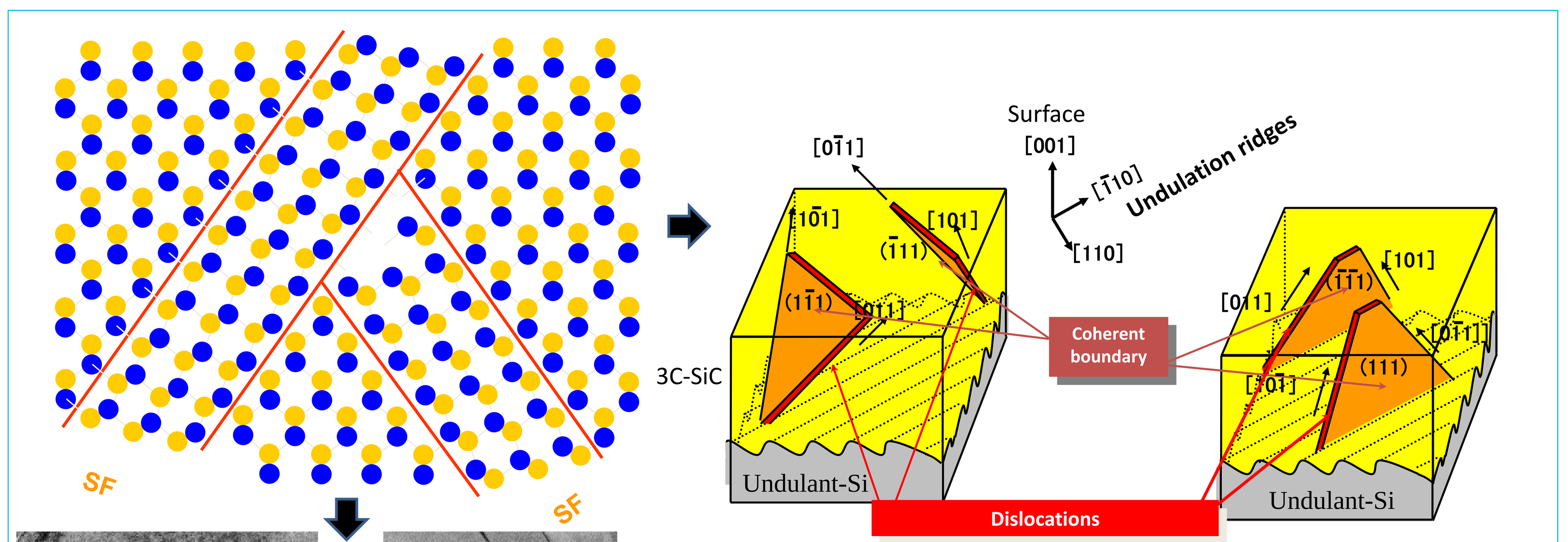
Goal: Analyze forest dislocation density as compared to the SF density in 3C-SiC (001).

Applications



- Durability in a large range of chemical, thermal, and electrical properties
- Highest saturated electron drift velocity
- Low density of states at 3C-SiC/SiO2 interface
- Favorable choice for use as a semiconductor in MOSFETs at voltages ranging from 600V-1200V [4]

Stacking Faults and Partial Dislocations

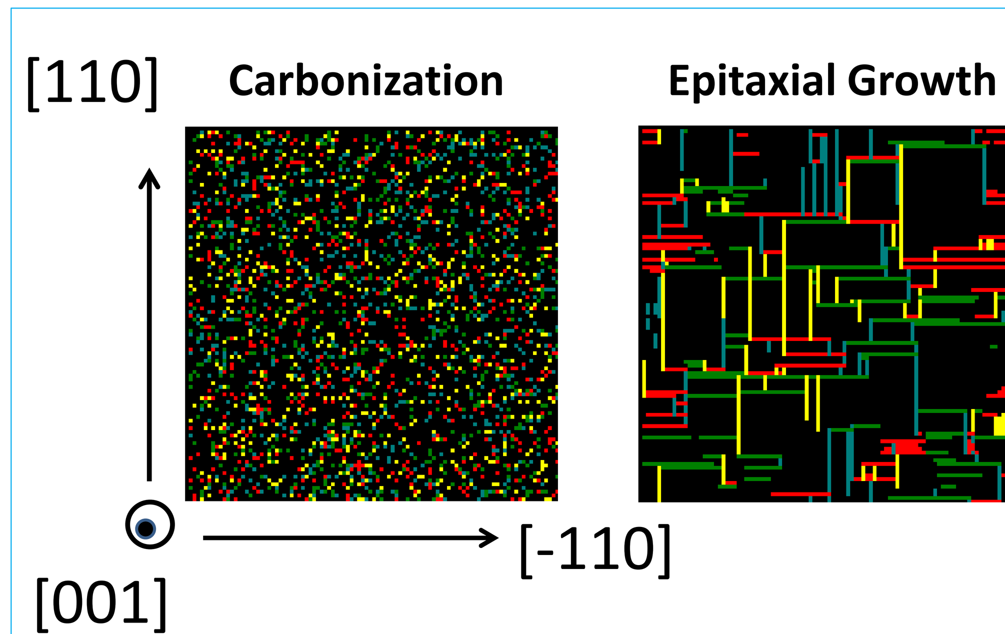


SF region parallel with (1-11) and (-111) planes

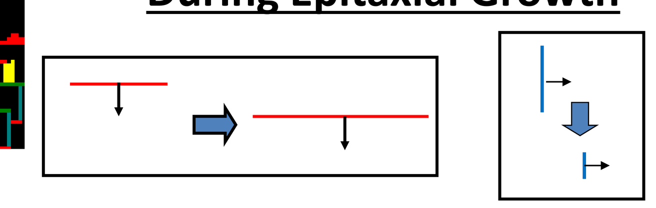
SF region parallel with (111) or (-1-11)

[H. Nagasawa]

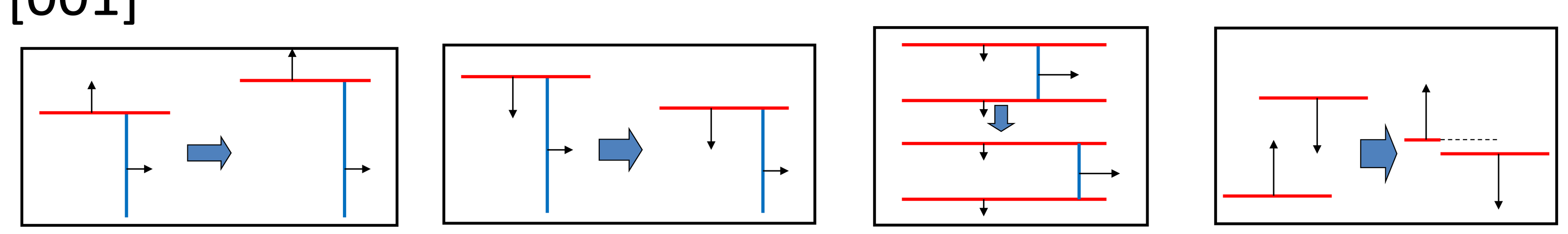
3C-SiC (001) Monte Carlo Simulation Geometry



Stacking Fault Interactions During Epitaxial Growth



Self expansion mode Self shrinking mode



Interactive stretching mode Interactive shrinking mode Drag mode Annihilation mode

Static Generation Probability of SFs:	12.5%	Annihilation Balance:	50/50	SiSF Expansion Probability:	12.5%	Angle Offset:	0.125°

Post-Epitaxial Growth

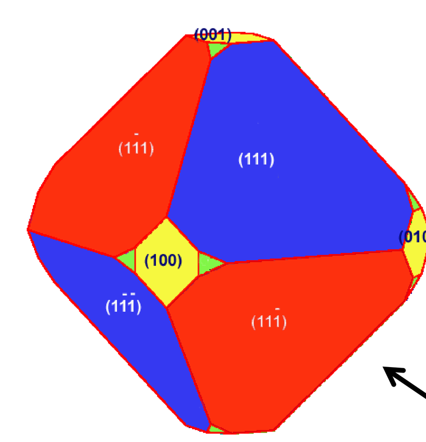
Burger's Vector for Gliding Partial Dislocations:

$$b_{90} = \frac{a}{6}[\bar{2}11] \qquad b_{30} = \frac{a}{6}[1\bar{2}\bar{1}]$$

$$b = b_{30} + b_{90}$$

$$b = \frac{a}{2}[\bar{1}10]$$

Burger's vector is decomposed into the 90° and 30° partial Burger's vectors



[H. Nagasawa]

Si-Core AE <<< C-Core AE:

Si-Core gliding velocity is several orders of magnitude higher: Can be omitted from simulations

b_{30} vector is projected onto the four equivalent planes corresponding to the four different types of SFs

Stress vector in [110] direction projected onto new gliding vectors

b30 = C-core Partial Dislocations → Edges of CSFs and SiSFs

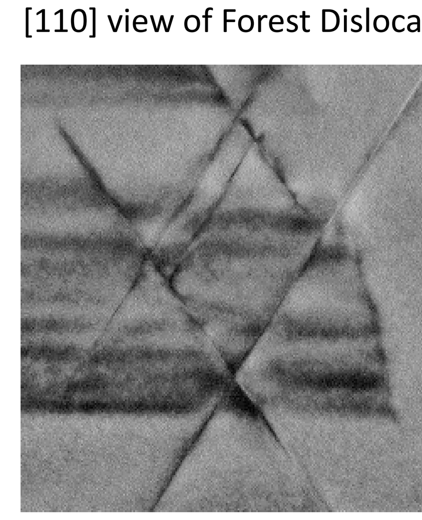
b90 = Si-core Partial Dislocations → Top edges of CSFs and SiSFs

Stress Applied To System:

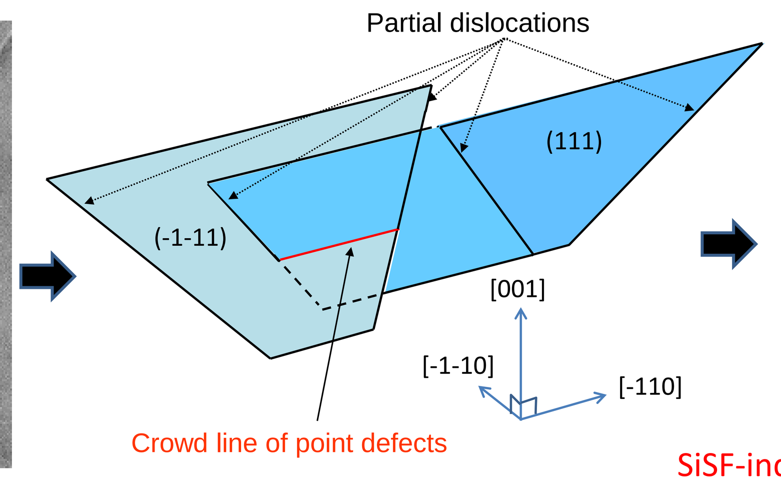
Stress is defined by the probability that the partial dislocation will glide in a given iteration of the simulation: 0% - 100% → 10% interval

Forest Dislocations

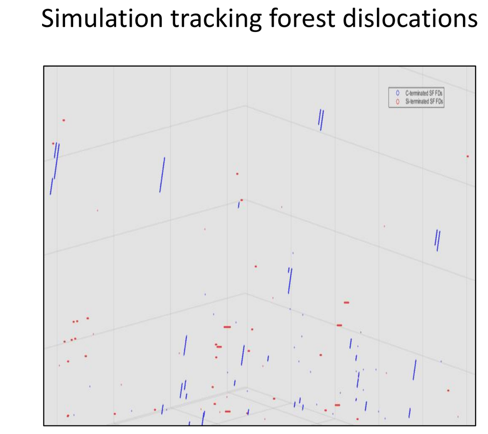
[110] view of Forest Dislocation



50nm [3]

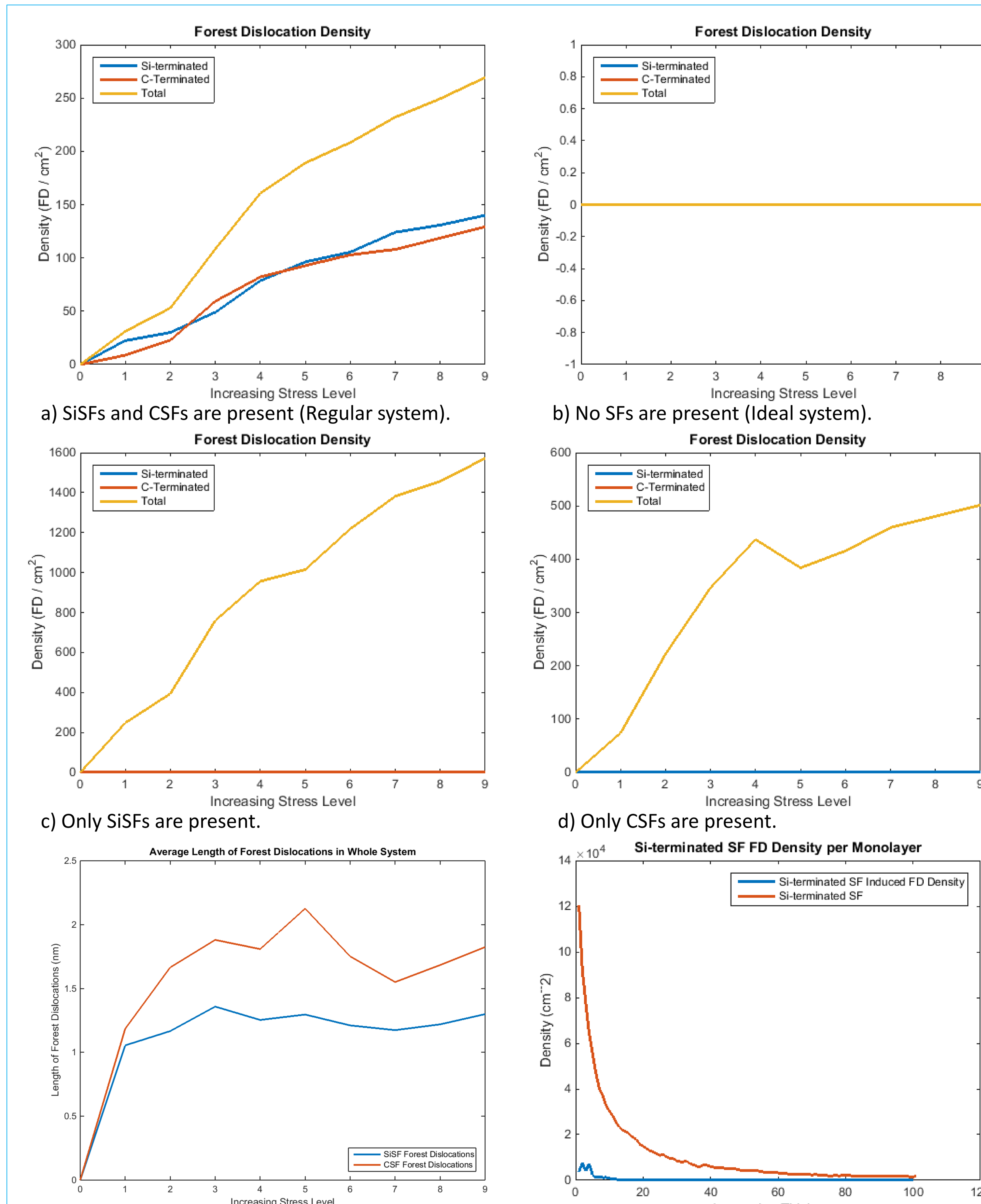


Simulation tracking forest dislocations



SiSF-induced FDs point in [110] direction
CSF-induced FDs point in [0-11] direction

Forest Dislocation and Stacking Fault Densities



a) SiSFs and CSFs are present (Regular system). b) No SFs are present (Ideal system). c) Only SiSFs are present. d) Only CSFs are present. e) SiSFs and CSFs are present f) SiSFs and CSFs are present

All data was obtained from simulations modeling a material of 30nm x 30 nm x 15nm in a length of 1000 time steps

Future Work

Define the activation energy of partial dislocations as a function of the temperature of the system and the area of the respective SF. Compare the simulation results to experimental results in order to have a clear insight into the mechanisms by which the generation of FDs affects the leakage current density.

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References

1. Y. Sun, S. Izumi, S. Sakai, K. Yagi, H. Nagasawa, Computational Materials Science 79 (2013) 216-222.
2. T. Kawahara, N. Hatta, K. Yagi, H. Uchida, M. Kobayashi, M. Abe, H.Nagasawa, B. Zippelius, G. Pensl, Materials Science Forum Vols. 645-648 (2010) 339-342.
3. H. Nagasawa, R. Gurunathan, M. Suemitsu, Materials Science Forum Vols. 821-823 (2015) 108-114.
4. H. Nagasawa, M. Abe, K. Yagi, T. Kawahara, Silicon Carbide, Vol. 1: Growth, Defects, and Applications (2010) 95-113.