Kinetics of surface instabilities and extended defects during the epitaxial growth of cubic silicon carbide

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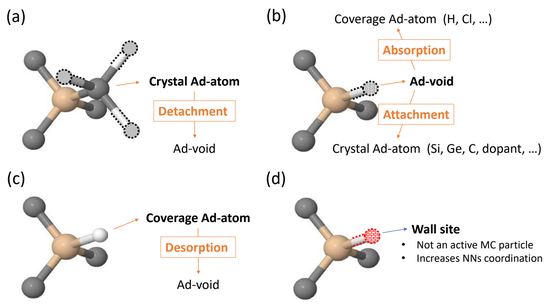
Introduction

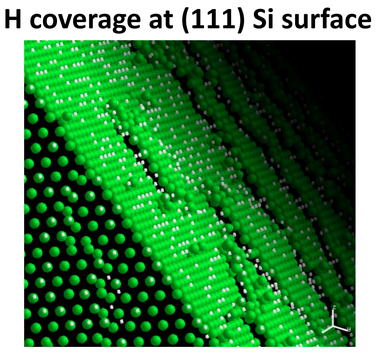
Emerging wide bandgap semiconductors like Silicon Carbide (SiC) or Gallium Nitride (GaN) have the potential to revolutionize the power electronics industry through faster switching speeds, lower losses, and higher blocking voltages, which are superior to standard silicon-based devices. The growth of high-quality substrates is a topic of extreme technological interest due to the importance of such materials for current and future technologies.
In our work [1] we focused on the atomic mechanisms ruling the extended defect kinetics in cubic SiC (3C-SiC), manifesting both stacking and anti-phase instabilities.

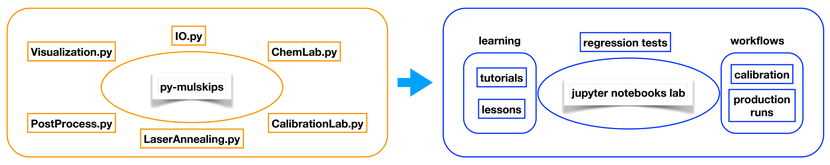
MulSKIPS simulation code

MulSKIPS [2,3] is a Kinetic Monte Carlo super-Lattice code, designed to study with an atomic resolution the growth kinetics of elements, alloys and compounds characterized by the sp^3 bond symmetry like Si, Ge, SiC and GaN crystals or the SiGe alloys. The code is able to simulate growth processes driven by Physical Vapor Depositions or Chemical Vapor Deposition.

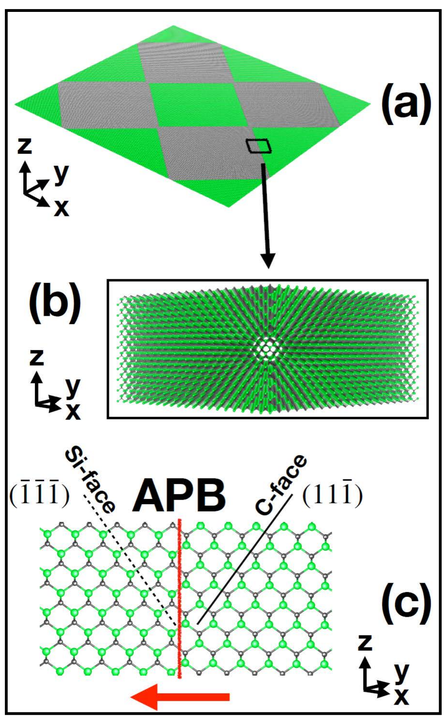


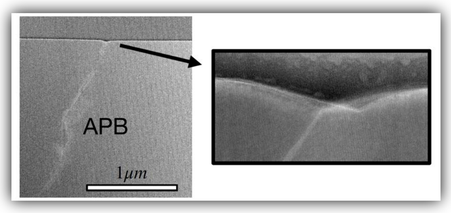
H coverage at (111) Si surface

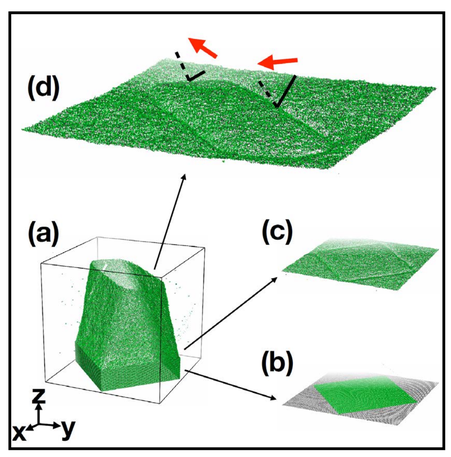




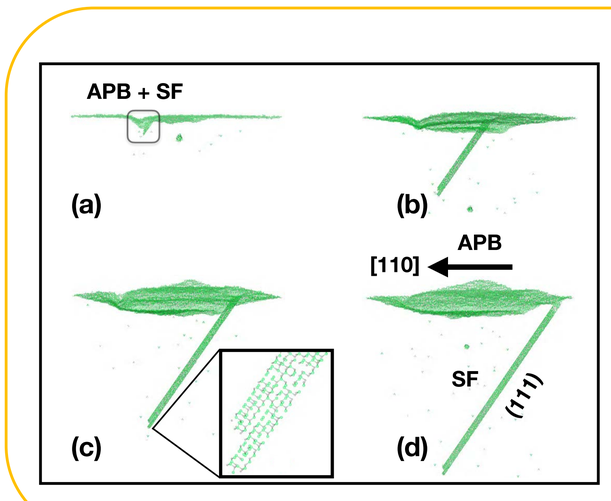
Anti-Phase Boundaries (APB) Kinetics

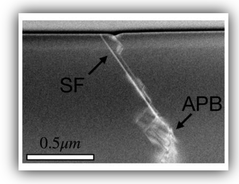




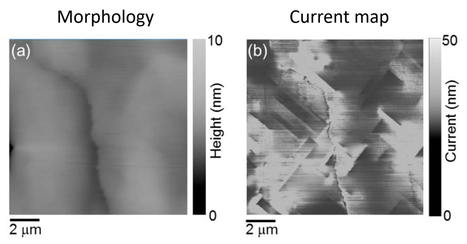


Triple Stacking Fault (SF) generation by APB

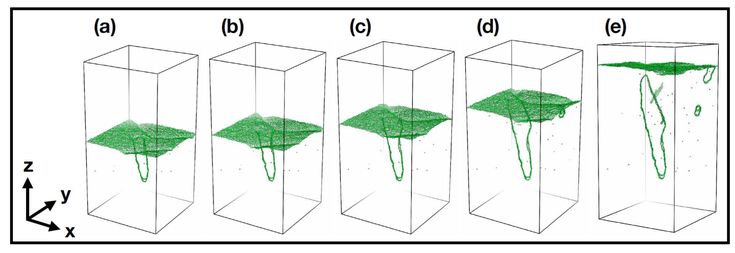


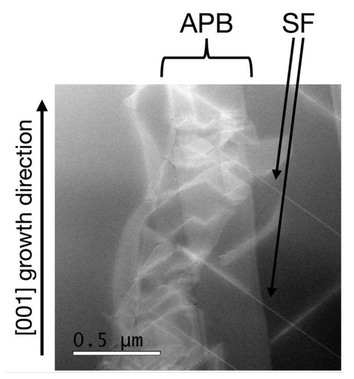


Conductive Atomic Force Microscopy



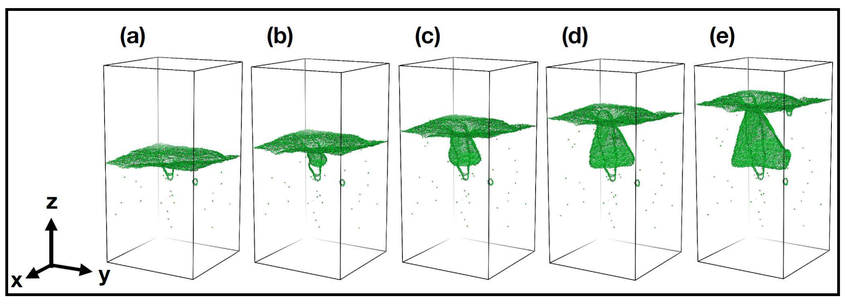
Stacking fault growth termination by APB

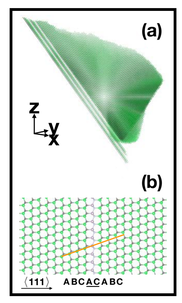




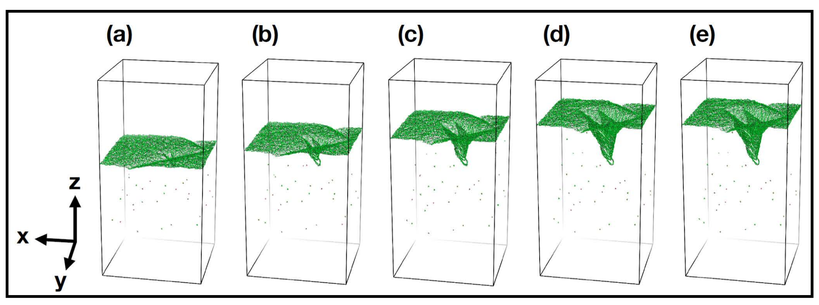
Single and multiple-triple SFs

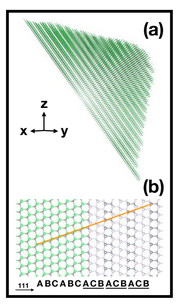
Generation and bulk growth of a single SF





Multiple sequence of triple SFs





Conclusions:
We have demonstrated that the long time kinetics of a really complex system can be predicted and analysed with atomic resolution. The processing of a defective system does not provide univocal upshots: this branching is ”intrinsic” and not dependent on the possible experimental variance of the initial state. Anti-Phase Boundaries are a critical source of other extended defects like SFs.

Acknowledgments
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References:
[1] G. Fisicaro, C. Bongiorno, I. Deretzis, F. Giannazzo, F. L. Via, F. Roccaforte, M. Zielinski, M. Zimbone, and A. L. Magna, *Appl. Phys. Rev.* **7**, 021402 (2020) **Featured Article**.
[2] A. La Magna, A. Alberti, E. Barbagiovanni, C. Bongiorno, M. Cascio, I. Deretzis, F. La Via, and E. Smecca, *Phys. Status Solidi A* **216**, 1800597 (2019).
[3] See code web page at github: https://github.com/giuseppefisicaro/mulskips where a user manual and regression tests for developers can be additionally downloaded.