Comprehensive Crystallographic Investigation of Diverse Structural Defects and Their Evolution Mechanisms in 4H-SiC for High-Reliability Power Devices

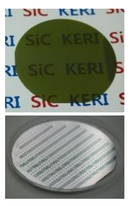
Moonkyong Na, Korea Electrotechnology Research Institute, Email: **nmk@keri.re.kr**

Why Stacking-Fault Identification Matters in SiC Power Devices

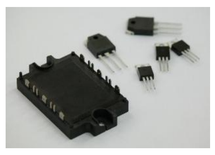
From wafer-scale defect signatures to atomic structure, defect evolution, electronic properties, and device impact

SiC for High-Power Applications

SiC Wafers and Power Devices



Power Module



Electric Vehicles

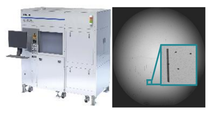


High-Voltage Power Grids

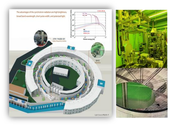


Multi-Scale Defect Analysis

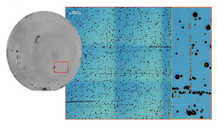
PL mapping



X-ray topography



KOH etching



FIB, HAADF HR-STEM



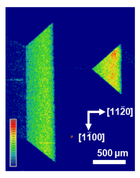
DFT calculation

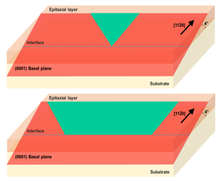


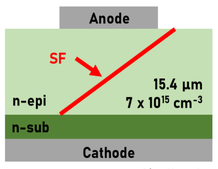
4H-SiC is a key material for high-efficiency, high-voltage power electronics, but stacking faults can propagate into device active regions and affect current conduction and reliability.

Wafer-scale PL → defect localization → atomic-scale structure → energetics & electronic structure → device impact

Research Strategy



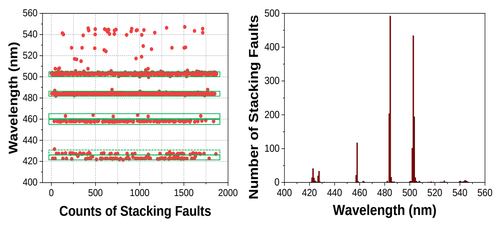




Directly correlate wafer-scale optical signatures with atomic-scale SF structures, energetics, and electronic properties to identify defect types, resolve complex configurations, understand their structural evolution, and assess their impact on device performance.

1. Wafer-Scale SF Identification by Direct PL–HR-STEM Correlation

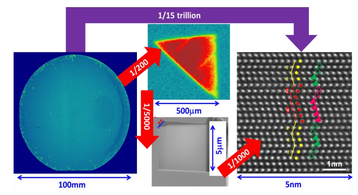
PL Spectra and Wavelength Distribution of SFs



~50,000 SFs / 70 wafers

Distinct PL Wavelength Bands

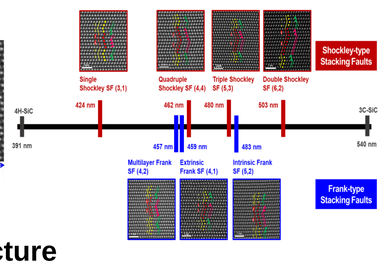
Direct 1:1 PL–HR-STEM Correlation of the Same SF



Same SF:

PL signature ↔ atomic structure

Characteristic PL Wavelengths of Seven Representative SF Types



Key Finding: Wafer-scale PL statistics enabled systematic SF classification, while direct 1:1 PL–HR-STEM correlation established structure-validated optical fingerprints for representative SF types.

Main Results

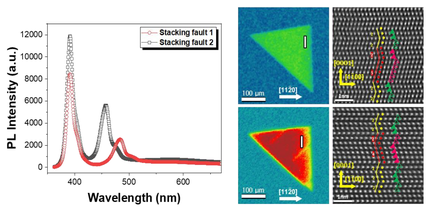
- ~50,000 SFs in 70 commercial 4H-SiC epitaxial wafers were statistically analyzed by wafer-level PL mapping.
- Most SFs converged into distinct PL wavelength bands with deviations below 0.5 nm, independent of wafer manufacturer.
- Direct PL–HAADF HR-STEM correlation established representative wavelength–structure relationships, which were subsequently expanded to seven representative SF types.

Technical Significance: Establishes a wafer-scale, structure-validated framework for SF classification and provides the foundation for a seven-type wavelength–structure map in 4H-SiC.

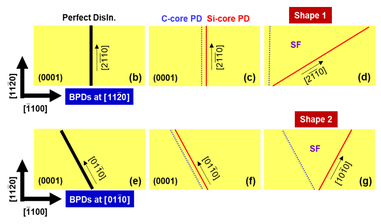
Mater. Sci. Semicond. Process. 175, 108247 (2024)

2. SF Shape Is Governed by Partial-Dislocation Geometry, Not SF Type

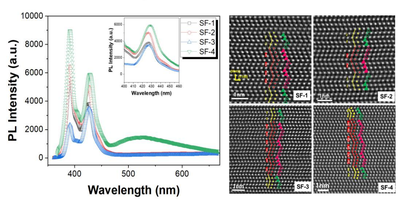
Broad Triangular Frank-Type SFs Confirmed by PL–HR-STEM



SF Shape Governed by Bounding Partial-Dislocation Directions



Different SF Structures with Nearly Identical PL Wavelengths at 427–428 nm



Key Finding: Broad triangular Frank-type SFs demonstrate that plane-view SF shape is not a unique signature of SF type; instead, SF morphology is governed by the geometry of the bounding partial dislocations.

Main Results

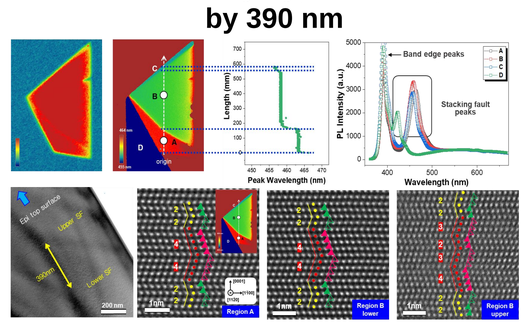
- Broad triangular (5,2) and (4,2) Frank-type SFs, previously associated mainly with Shockley-type SFs, were directly confirmed by HAADF HR-STEM.
- The triangular shape can be explained by the preferred directions of the partial dislocations bounding the SF, rather than by SF type alone.
- Four distinct Shockley- and Frank-type SF structures exhibited nearly identical PL wavelengths of 427–428 nm, showing that PL wavelength alone is also insufficient for unique identification.

Technical Significance: Demonstrates that neither plane-view SF shape nor PL wavelength alone uniquely determines SF type, establishing the need for direct crystallographic confirmation for reliable SF identification.

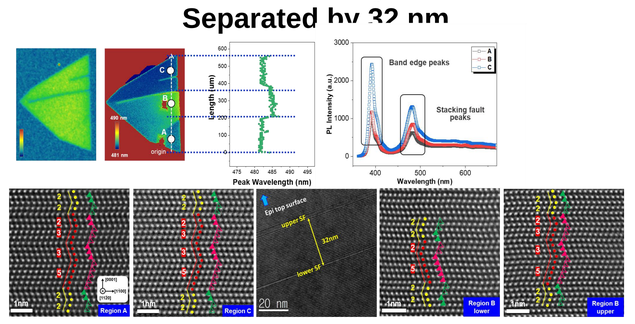
Appl. Phys. Lett. 124, 152109 (2024)

3. First Direct Identification of Overlaid SFs Along the Growth Direction

Overlaid Shockley-Type SFs Separated by 390 nm



Overlaid Frank-Type SFs Separated by 32 nm



Key Finding: PL spectral line scans resolved multiple emission components within apparently single SF features, while HAADF HR-STEM directly confirmed multiple SFs overlaid at different depths along the growth direction.

Main Results

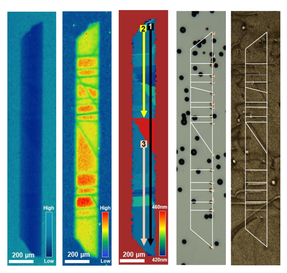
- Overlaid SSFs were resolved as lower 4SSF (4,4) and upper SSF (4,3,2,3), separated by 390 nm along the c-direction.
- Overlaid FSFs were resolved as lower FSF (5,2) and upper FSF (5,3,3,2), separated by only 32 nm.
- The SSF (4,3,2,3) was identified for the first time with a characteristic PL wavelength of 456 nm, while the FSF (5,3,3,2) PL wavelength was determined as 481 nm.

Technical Significance: Demonstrates that a single plane-view PL feature can conceal multiple SFs at different depths, showing that reliable SF identification requires depth-resolved structural correlation beyond plane-view PL analysis.

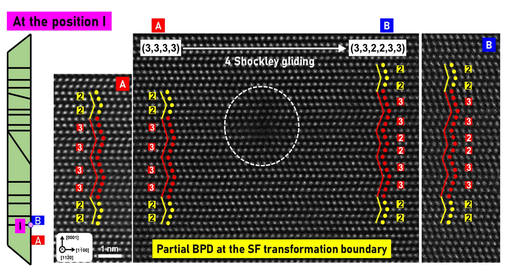
Appl. Surf. Sci. 703, 163425 (2025)

4. First Identification of Internal Line Features and SF Transformation Mechanism in Trapezoidal Defects

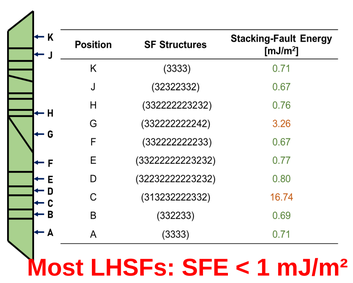
First Identification of Internal Line Features as Partial BPDs



Direct Observation of Local SF Transformation



DFT: Exceptionally Low SFEs of Large-Height SFs



Position	SF Structures	Stacking-Fault Energy [mJ/m²]
K	(3333)	0.71
J	(32322332)	0.67
H	(332222223232)	0.76
G	(332222222242)	3.26
F	(332222222233)	0.67
E	(33222222223232)	0.77
D	(32232222223232)	0.80
C	(313232222332)	16.74
B	(332233)	0.69
A	(3333)	0.71

Most LHSFs: SFE < 1 mJ/m²

Key Finding: Internal line features in trapezoidal defects were identified as partial BPDs at local SF transformation boundaries. DFT revealed exceptionally low SFEs for most large-height SFs, providing a thermodynamic basis for their structural transformations.

Main Results

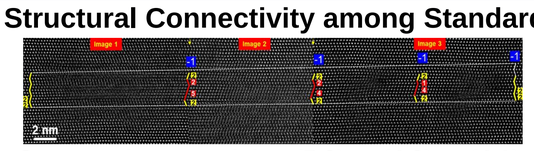
- Internal PL line features were identified as partial BPDs accompanying local SF transformations.
- Atomic-resolution HR-STEM directly revealed transformations among large-height Shockley-type SFs, including intermediate structures.
- Most LHSFs exhibit very low SFEs (< 1 mJ/m²); together with small energy differences and facile SPD glide, these factors enable multiple transformations under growth-induced driving forces.

Technical Significance: Reveals the previously unresolved internal architecture of trapezoidal defects and establishes a crystallographic–thermodynamic mechanism for SF evolution in 4H-SiC.

Acta Mater. 315, 122392 (2026)

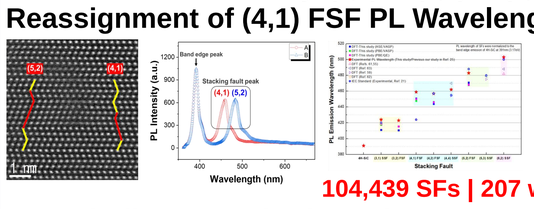
5. Unified Framework for Frank-Type Stacking Faults

Structural Connectivity among Standard



Structural connectivity: (5,2) — (4,2) — (4,1)

Reassignment of (4,1) FSF PL Wavelength



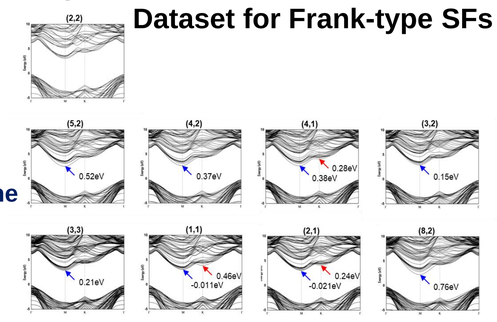
Reassignment of the standard (4,1) FSF

(4,1) FSF:

424 nm ➔ 459 nm

104,439 SFs | 207 wafers

Comprehensive Electronic-Structure Dataset for Frank-type SFs



Key Finding: Standard Frank-type SFs are structurally connected within a common crystallographic framework, and the characteristic PL wavelength of the (4,1) FSF is established as 459 nm, revising the long-accepted 424 nm assignment.

Main Results

- Atomic-scale observation revealed structural connectivity among standard (5,2), (4,2), and (4,1) FSFs.
- Intrinsic/extrinsic character is determined by the final crystallographic topology rather than simple layer insertion or removal.
- Electronic-structure calculations clarified their defect states, while HR-STEM/PL correlation identified the standard (4,1) FSF emission at 459 nm, calling for reconsideration of the 424 nm assignment in the IEC standard.

Technical Significance: Establishes a unified crystallographic–thermodynamic–electronic–optical framework for identifying and interpreting Frank-type SFs in 4H-SiC.

Acta Mater. 321, 122747 (2026)

From Stacking-Fault Structure to Device Reliability

- **Together, these studies demonstrate that stacking faults cannot be reliably identified or understood from a single observable such as PL wavelength or plane-view morphology.**
- **Correlating wafer-scale PL signatures with atomic-scale crystallography, three-dimensional defect configurations, transformation energetics, and electronic structure establishes a structure-based framework for assessing defect behavior and its impact on 4H-SiC power-device performance and reliability.**
- **This framework is being extended to direct device fabrication and electrical characterization to quantify defect-induced performance degradation.**

2026 Masao Horiba Awards — Honorable Mention, October 15, 2026