# Impact of Grain Boundaries on Functional Properties of Silicon Solar Cell Absorbers

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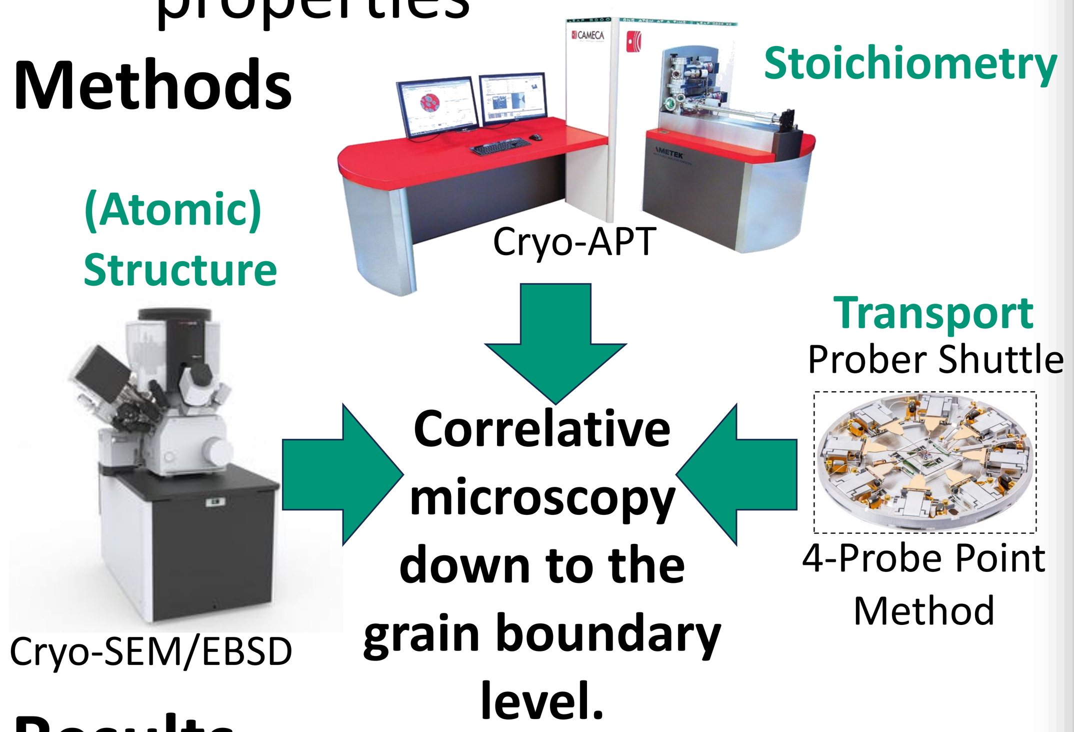
## Introduction

- Silicon absorbers foundational to PV tech
- Bulk crystal quality often primary focus, Grain boundaries (GBs) influence device performance as well
- Thin-film cells: small grain sizes and high GB density.
- Correlation of atomic structure and chemistry of Si GBs with electronic properties

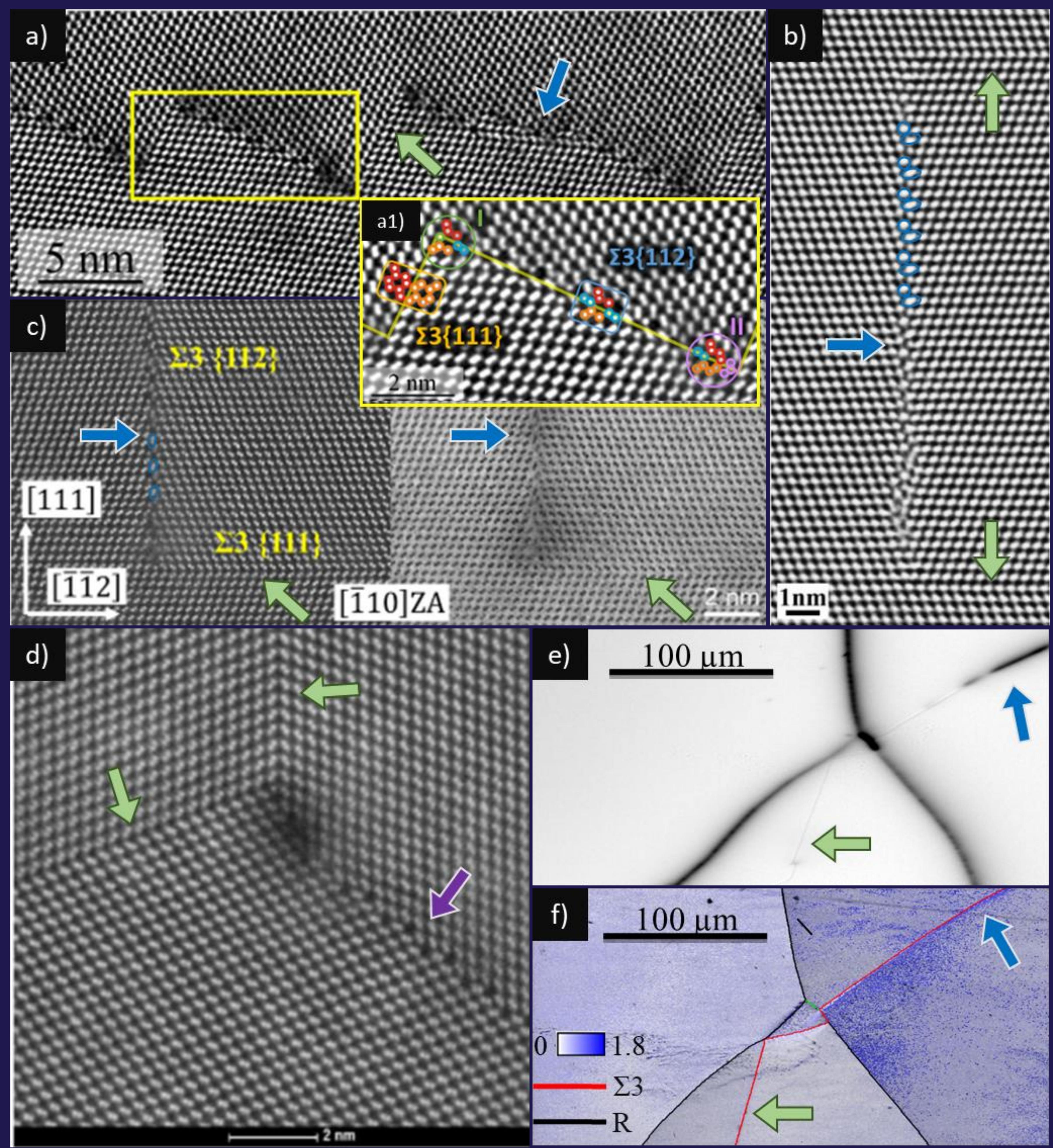
## Methods

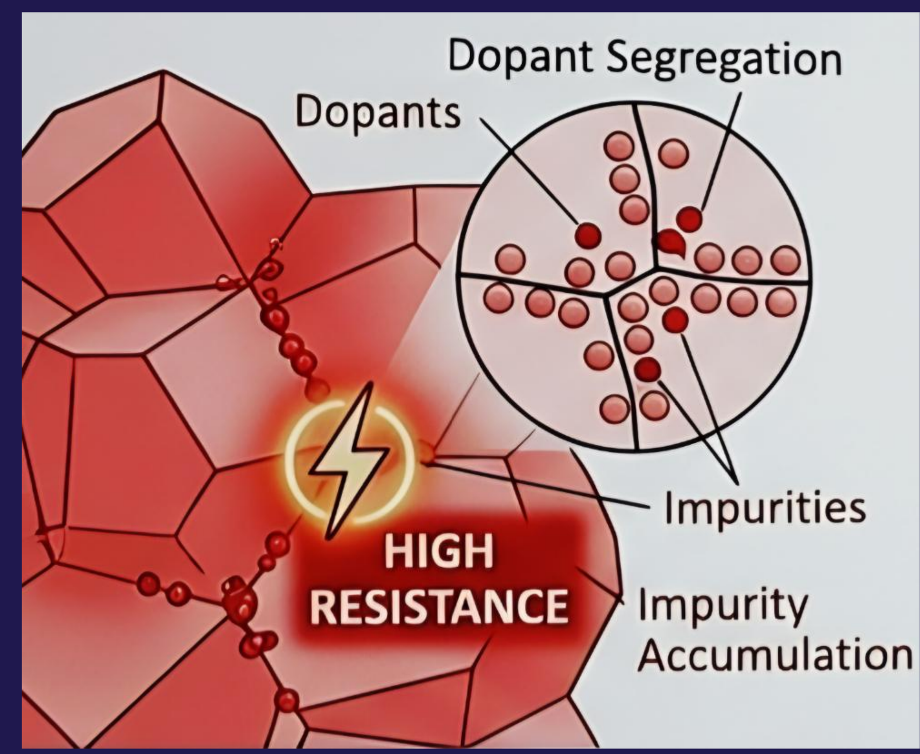



## Results

- Coherent Σ3 {111} twins: Negligible recombination activity.
- Σ3 {112} GBs: Medium recombination activity.
- Random high-angle GBs (RHAGB) & Σ9 interfaces: High recombination activity

# The impact of a GB on efficiency is directly tied to its symmetry and coherence.




Mechanisms which make GBs detrimental:

- Impurity segregation: O and C accumulate at GBs, increasing recombination activity.
- Charge defects: Formation of charged vacancies creates deep electronic states within the band gap.
- Barrier heights $\phi$: Si GBs exhibit positive barrier heights, creating a potential barrier for charge carriers.

Atomic structures of several grain boundaries in silicon. The {111} Σ3 GBs are indicated with light green arrows, while {112} Σ3 GBs are shown using a blue arrow and Σ9 by a purple arrow. (a)-(d) HAADF and BF-STEM images of GBs (e) EBIC map of an area of multicrystalline Si (f) SEM image of the sample area in (e) overlaid with EBSD information on GB crystallography.[1,2]

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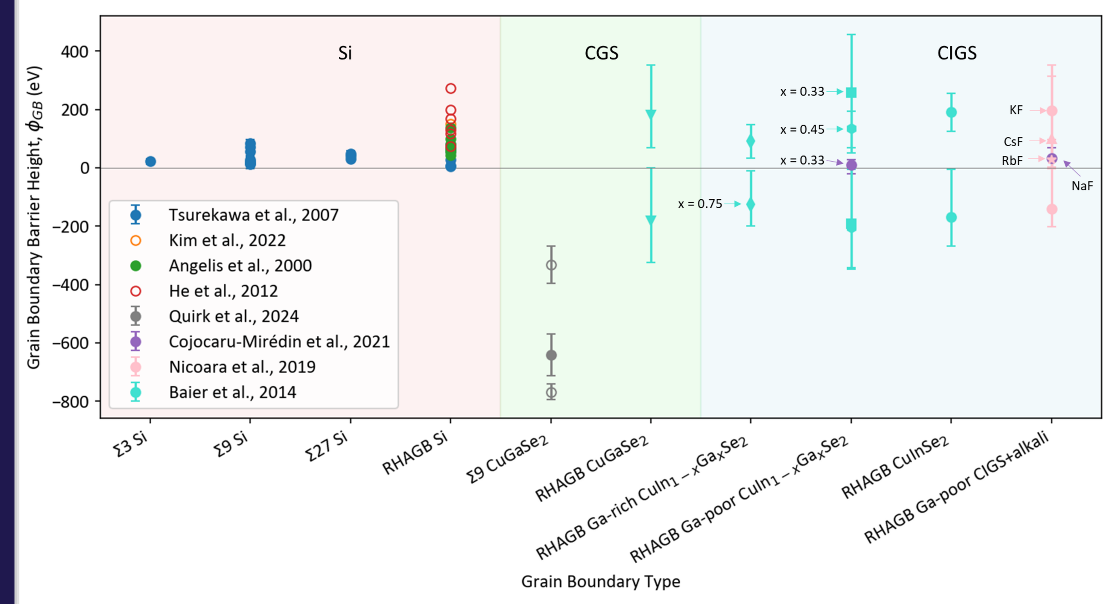
## Results




Grain-boundary barrier height $\phi_{GB}$ of Si and CIGS, dependent on their Σ-type and composition.[1,3]

## Conclusions

Strategies to improve the power conversion efficiency of thin-film Si cells by lowering the potential barrier height $\phi$:

- Morphological control: Controlled nucleation and post-deposition annealing; bigger grain size and formation of low-Σ GBs.
- Chemical purification: Reduction of O and C concentrations to mitigate sink effect of GBs.
- Interface neutralization: Passivation techniques (e.g., H) neutralize localized charges and reduce potential barrier height.

Systematic, rational GB engineering could enhance charge collection and mitigate ion-induced degradation, raising the efficiency of thin-film Si solar cells.

## References

[1] O. Cojocaru-Mirédin et al., MRS bulletin 51, 189 (2026).

[2] A. Stoffers, Korngrenzensegregation in multikristallinem Silizium, RWTH Aachen University, 2017.

[3] S. Tsurekawa et al., Materials Science and Engineering: A 462, 61 (2007).