Renewable Energy Research Center

Achievable performance improvements for solar cells through detailed analysis of concealed interface mechanisms

Jonathon Mitchell
National Institute of Advanced Industrial Science and Technology
Renewable Energy Research Center Photovoltaic Power Team

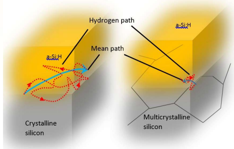
Research Objectives

Identify underlying mechanisms which influence the overall performance of photovoltaic devices.

Hydrogen previously shown to follow influenced multipath process prior to passivation of deep-defects.

PTS-MESH algorithm developed: Iterative substructuring methods, induced dimension reduction, quasi minimal residual, generalized minimum residual

Using PTS-MESH we enable particle tracking within interface regions on both planar (single crystal silicon) and dislocated surfaces (multi-crystalline silicon).



Experimental Details

Intensity of electric field

$$E = \frac{p}{4\pi\epsilon_o R^3}(a_R\cos\theta + a_\vartheta\sin\theta)$$ for single particle

$$E = \frac{p}{4\pi\epsilon_o R^3}\oint_{S_1}^{S_2}(a_R\cos\theta + a_\vartheta\sin\theta)\,dS$$ for surface space

Displacement of field

$$D = \frac{a_R}{R}\int_{S_1}^{S_2}(a_R\cos\theta + a_\vartheta\sin\theta)\,ds: dS$$

Polarisation of field

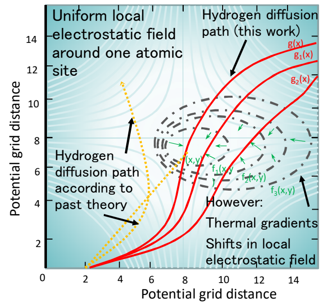
$$p = a_2 4\pi\epsilon_0 b^3 E_v \qquad dV = \frac{p.a_R}{4\pi\epsilon_0 R^2}dv$$

E = Electric field intensity (V/m) a_R/a_ϑ =

D = displacement gradient θ = vector component

p = polarisation gradient dS/ds = surface space (2d/3d)

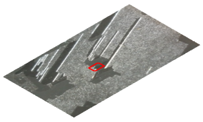
R = resultant vector dV = voltage

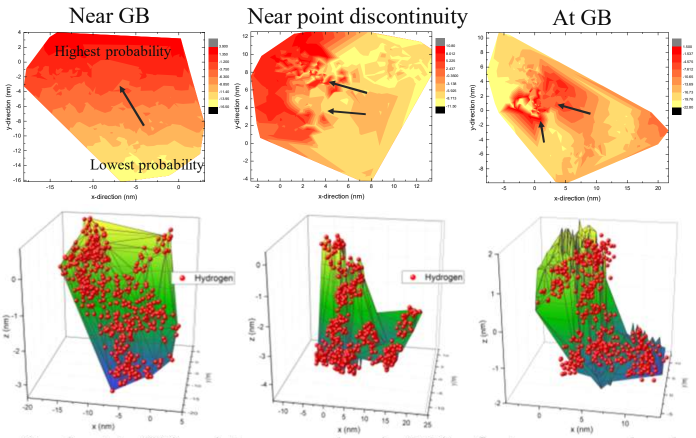


Results

Hydrogen diffusion over dislocation

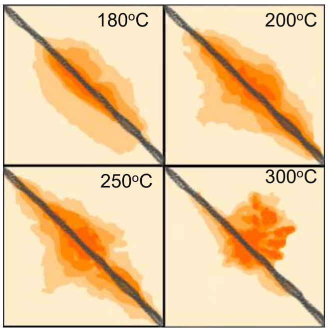
- Nearest neighbour potential approximation for interstitial hydrogen in the transport level, following least-action principles, reveals a 3 dimensional free path.
- Up to 4 million Lagrangian points are evaluated within each potential Eulerian grid.
- Boundary conditions are accumulated by interpolation.
- When aggregated, the potential probability distribution can be determined.





- Steady-state (SS) and Frequency-domain (FD) reflectance are analysed in tandem to obtain broad wavelength coverage with accurate depth penetration for multicrystalline surfaces.

Penetrative transport paths on structural discontinuities



Lower temperatures: Favourable distribution along grain boundary.
Higher temperatures: pseudo-spore motilities increase, preferential boundary transport diminished.

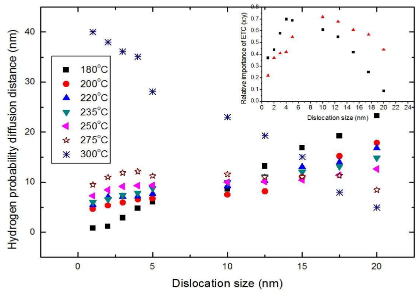
Aggregated hydrogen probability distribution* across extended dislocation (grey line) between two crystal grain boundaries shown in 2D-space for discrete time interval at different temperatures.

* Observed strong probability profiling removed

Hydrogen probability distribution distance for trans-dislocation mobility

Smaller dislocation sizes limit mobility to a few nanometre for lower temperatures, with mobility improving at dislocations above 10 nm.

(inset) the significance profile of the effective thermal conductivity relative to grain boundary geometry.



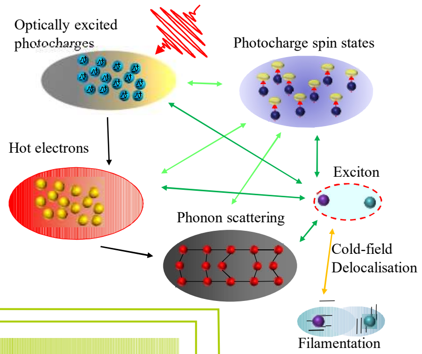
Observed crossover point at approximately 8-10 nm suggests that thermal characteristics are significant, and that intergranular properties may change.

Discussion

The effective electronically relevant width of a dislocation is larger than its geometric dimensions, therefore, phonon scattering is a likely determinant of mitigating boundary diffusion.

Detailed particle tracking with electrostatic field metrology.

Microscopic mechanisms leading to these ultra-fast processes are still not clear.



Molecules of dielectric and semiconductors materials, like a-Si:H/SiN/SiO and crystalline silicon, are often macroscopically considered neutral.

External and intrinsic electric field can lead to small displacements, resulting in:

- Enhanced or reduced coverage of electronic trapping sites.
- Changes in thermal conductivity.
- Shifts in optical mutability.

Quasi-particle processes and spin-state complex can be detected for ultrashort (fs) times.

Summary

Demonstrated suitable residual minimisation at all tested mc-Si surfaces.
Additional processes, phenomena and their interaction influence the final performance of fabricated devices.
The electronic performance and thermal conductivity can be modified.

Reference

Adaptive Particle Tracking of Hydrogen within the a-Si:H/c-Si Interface Using PTS-MESH for Planar and Dislocated Surface, J. Mitchell, 26th PVSEC (2016).