Renewable Energy Research Center

Adaptive Particle Tracking of Hydrogen within the a-Si:H/c-Si Interface

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研究の目的

Hydrogen distribution on the depositing surface is often views as a Gaussian probability distribution.

- Overlooks nearest neighbour boundary conditions,
- Small scale turbulence.

The resulting is a poor understanding of hydrogen passivation at the surface and within grain boundaries.

To better understand how hydrogen interacts with a c-Si surface interfaced with a-Si:H, a model involving domain decomposition was created which can interface a Eulerian grid with Lagrangian techniques to provide an adaptive moving-mesh in Eulerian space with Lagrangian point-aggregation for an 864 site surface.

実験

Eulerian grid – considers the rate of change of system variables at a particular point in space.
Lagrangian techniques – tracks individual particles along their trajectories.
At defined increments in time, the point where a particle originated from is determined, while interpolation estimates the value of dependent variables at grid boundaries surrounding the point the particle originates from.

Global Point model

$$\underbrace{\frac{DF}{Dt} = \frac{dF}{dt}}_{\text{Eulerian rate-of-change}} + \underbrace{\left(v \cdot \vec{\nabla}\right)F}_{\text{Advection term}}$$

Particle state

$$\frac{DV}{Dt} = S(V)$$

V (dependent variable)

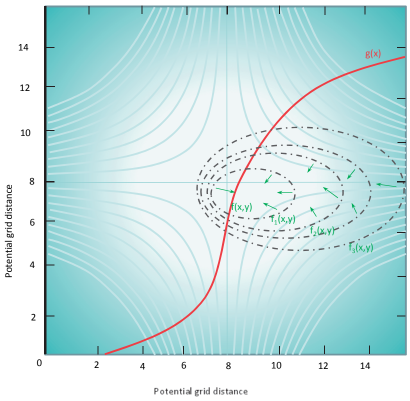
- velocity,
- Energy,
- State

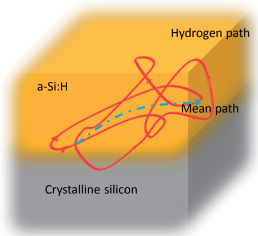
Determination of the curvature probability

$$\frac{1}{r} = \sqrt{\left(\frac{d^2x}{ds^2}\right)^2 + \left(\frac{d^2y}{ds^2}\right)^2}$$

Probabilistic refinement is utilised to improve the efficiency of this method by filament reduction.

結果





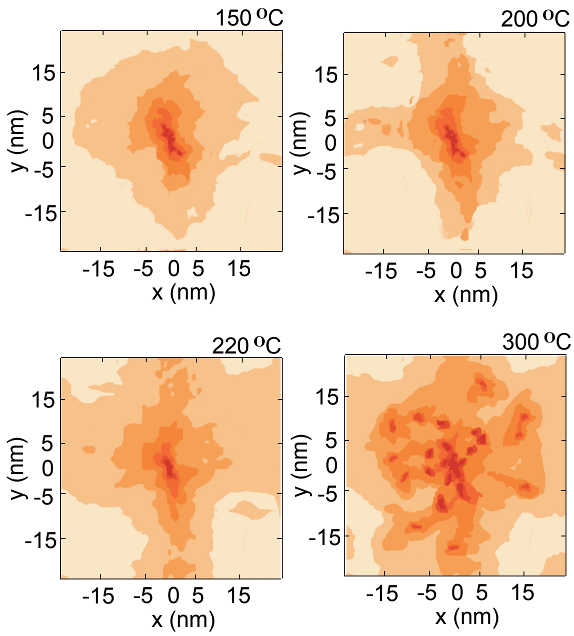
Euler-Lagrange equation: (L_x and L_v denote partial derivatives of L)

$$L_x(t, q(t), \dot{g}(t)) - \frac{d}{dt} L_v(t, q(t), \dot{g}(t)) = 0$$

- 2.5 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.
- Increases in temperature (150°C to 300°C) shows higher probability of target Hydrogen migrating across the c-Si surface.
- At 300°C, multiple target interaction occurs reducing confidence in particle tracking, however, the system variable rate of change remains.

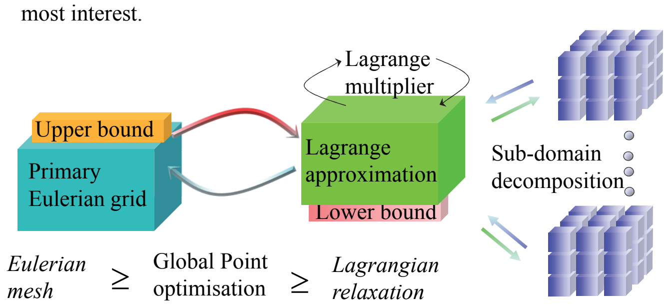
- Nearest neighbour potential approximation for interstitial hydrogen in the transport level, following least-action principles, reveals a 3 dimensional free path.

Probability Distribution of transport Hydrogen



考察

- Solving a boundary value problem by separating into smaller boundary value problems on subdomains and iterating to coordinate the solution between adjacent subdomains.
- Smoothed particle hydrodynamics can be evaluated with sharp discontinuities.
- Moving-mesh regions of highest resolution aligned to the regions of most interest.



結論

- Probabilistic refinement is utilised to improve the efficiency of this method by filament reduction.
- Iterative substructuring methods, induced dimension reduction, quasi minimal residuals and generalised minimum residuals.
- Steady-state (SS) and Frequency domain (FD) reflectance are analysed in tandem to obtain broad wavelength coverage with accurate penetration depth.
- Modelling of hydrogen transport along surface with penetrative transport paths on structural discontinuities like grain boundaries represents a challenge.
- Larger the variance, the more heterogeneities will distort the model predictions.

参考文献

Wang, H., Ewing, R., Qin, G., Lyons, S., Al-Lawatia, M., Man, S., “A family of Eulerian–Lagrangian localized adjoint methods for multi-dimensional advection-reaction equations”, Journal of Computational Physics, 152(1), (1996).