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Hybrid Quantum/Classical Molecular Dynamics for Impurity-Segregated Nanostructures

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Recent advances in parallel and GRID computing technologies have expanded the length scale of the systems dealt by molecular simulations upto angstroms. However, there are still difficulties in modeling the interactions between impurity atoms and nanoscale defects, and their effects on the macroscopic properties of nanostructured materials. We have been developing the hybrid quantum/classical molecular dynamics algorithm [1] to overcome the difficulties. In the method, the quantum cluster calculation, based on the tight-binding and/or the density-functional method, is applied locally to a chemically active region, and is coupled seamlessly to the nanoscale system modeled by a classical interatomic potential.

We apply the hybrid method to microscopic processes of hydrogen diffusion in a Si grain boundary [2]. Despite of its importance in semiconductor processes, the precise knowledge of hydrogen diffusion in silicon has not been precisely obtained yet. The diffusion constant depends strongly on temperature, not necessarily in a perfect Arrhenius manner. This is because hydrogen diffusion can be influenced sensitively by collective effects, low temperature quantum effects, impurities, defects, interfaces, etc. Here we focus on the effect of hydrogen-defect interactions in the diffusion process at finite temperatures.

Figure 1 illustrates the atomic configuration of a (001)Σ5 twist grain boundary (GB) of Si. This GB is known to have the large density of coordination defects, and hence it can be regarded as one typical structure of strong trapping site for hydrogen atoms in Si. The highlighted area with dashed circle in Fig. 1 indicates the QM cluster embedded in the GB region. Figure 2 depicts the trajectory of H atom together with average positions of the Si atoms in the QM region. The H atom is hopping along the GB plane at 1200K, whereas the H atom is strongly bonded to a coordination defect in the GB at the temperatures at and below 800K.

The hybrid method is also applied to study hydrogen/nickel segregated dislocation cores in diamond [3] and structure/stability of a dislocation in alpha-alumina. In the presentation, preliminary results on these systems will be reported.

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References

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[2] K. Tsuruta *et al*., *Mater. Sci. Forum* **539-543** (2007) 2804.
[3] K. Tsuruta *et al*., *Comp. Mater. Sci.* **38** (2007) 873.

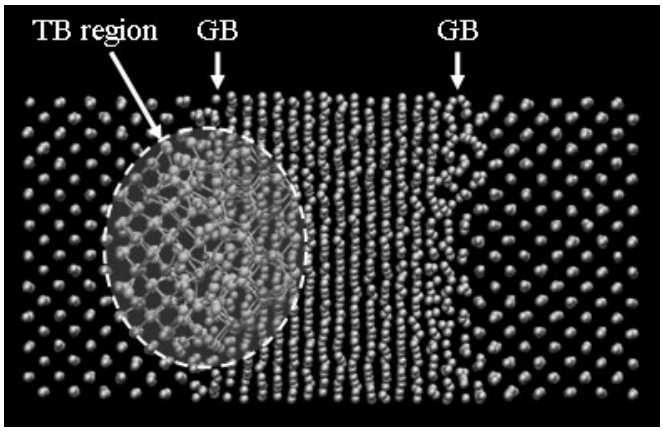

FIG 1. Atomic positions of (001)Σ5 twist grain boundary of Si with a H atom. "GB" and dashed circle indicate position of the grain boundary and region for TB-cluster calculation, respectively.

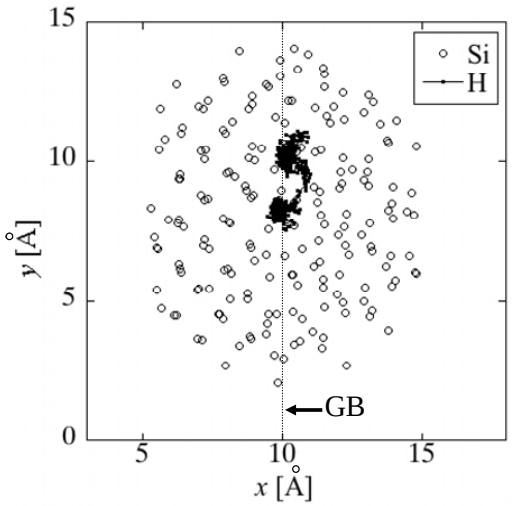

FIG 2. Trajectory of H atom in QM region of Si grain boundary at 1200K.