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Device Simulation using Symmetric Smoothed Particle Hydrodynamics

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Abstract content
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The real-space approach is widely used for electronic structure calculations. In particular, it is used for large systems, because a real-space mesh is suitable for large-scale parallel computing. The real-space approach also allows the capture of a clear physical image. For the simplest real-space implementation, the higher-order finite-difference method is used as a discretization technique. Besides, there are also meshfree methods as real-space implementations. These methods have an advantage in their non-uniform distribution of computation points, which also reduces computational costs.
As one of the meshfree technique, we have been studied Smoothed Particle Hydrodynamics (SPH) which is applied to the electronic structure calculation. SPH was originally developed for hydrodynamic problems, which deal with complex shapes, large deformations and free surfaces. It is a typical meshfree particle method, in which the system is represented by a finite set of arbitrarily distributed particles without using any mesh. However, SPH is known for its low accuracy. As one of alternatives, Symmetric Smoothed Particle Hydrodynamics (SSPH) is proposed. In this study, we have applied SSPH to the HEMT device simulation. In layered structures such as FET, the current density is mainly dependent on the electron mobility and the electronic field in the vicinity of the gate part, where both of them are recognized as a constant. With this approximation, the relation between the channel current and the gate applied voltage can be obtained by one dimensional calculation. Then, it is easier to confirm the device properties in the SSPH technique.
This study evaluates the accuracy of SSPH for this typical electronic structure calculation. The results are then easily compared to the finite-difference method. In this paper, we will demonstrate some of practical electronic structure calculations using non-uniformly distributed particles.

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