Development of high accuracy predicting technique of elemental diffusion in molten glass by molecular dynamics simulation

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Objectives

To obtain the required characteristics in industrial glass, it is important to control the diffusion of additional elements. Simulation of diffusion phenomenon is possible in principle using the molecular dynamics method. If the concentration of the additive element is low, to improve the statistical properties of the simulation analysis, it is necessary to scale-up the model. The purpose of this study is to investigate the possibility of accurately analyzing the diffusion of elements in the glass of a large-scale model by using a super computer.

Outline of Results

Using molecular dynamics simulator LAMMPS, an all atom classical molecular dynamics simulation was carried out. The intermolecular potential was adopted Born-Mayer potential. PPPM (Particle-Particle-Particle-Mesh) method was used in the calculation of the Coulomb force. Regarding the benchmark results, it was found that the execution time was minimal when using 3,072 nodes in 4 million atoms calculation, and that FFT communication time becomes a bottleneck when using the number of additional nodes. With respect to the relationship between the model size and accuracy of analysis of diffusion simulation, mean square displacement of the additional element by large-scale simulations of 600,000 atoms using K computer had better statistical properties, and it was confirmed that it improved the analysis precision of the diffusion coefficient.

The statistical accuracy of diffusion analysis was improved by the large-scale model

Relationship of the mean square displacement of the additive element and model size