V238-P015 **Room: Poster Session Hall** **Time: May 22**

Molecular dynamics simulations of a shock-tube experiment with a two-component Lennard-Jones particle system

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To investigate a rapid dynamics of a magma-gas mixture in a Vulcanian eruption, we do extensive molecular dynamics simulations.[1] For computational simplicity, we mimic a situation of shock-tube experiment and we model magma and gas components by Lennard-Jones particles having two set of parameters; The Lennard-Jones particle has an inter-particle interaction that is characterized by short range repulsion, midrange attraction and long range freedom. This feature makes the particles show several thermodynamic phases such as gas, liquid, solid and coexistence one. The molecular dynamics simulations enable us to study the dynamics in the context of nonequilibrium physics.

By extensive molecular dynamics simulations, the present microscopic model shows hydrodynamic behavior which is consistent with the result of one-component compressible hydrodynamic equations proposed by Woods.[2] In addition, we observe gas bubble nucleation in a saturated magma-gas mixture, growth of nucleated bubbles, and finally a transition from a bubbly magma flow to a magma dispersion flow. A quantitative analysis for magma cluster gives a power-law size distribution of magma cluster, which is frequently observed in cluster aggregation processes. One of advantages of microscopic modeling is all field quantities such as velocity, pressure, and stress tensors are easily calculated by the simulation. Results of a temperature field show that temperature inhomogeneity exists between magma droplets and gas bubbles. It means that a structural formation of a bubbly magma flow or a magma dispersion flow occurs under highly nonequilibrium conditions. It suggests a theoretical description by continuum modeling should describe such inhomogeneity.

[1] S. Yukawa and N. Ito, physics/0510147.

[2] A. W. Woods: Nucl. Eng. Design, 155 (1995) 345.