THE GEODYNAMICS SEMINAR

N°646

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Geodynamics Research Center

2025.12.12 (Fri.) 16:30 ~

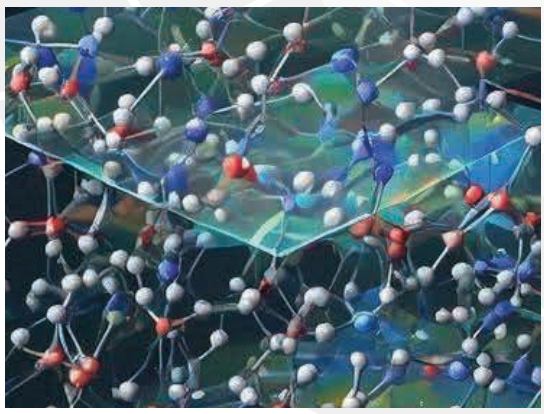
Venue: Meeting Room #486

Science Research Bldg. 1, 4th floor.

Ehime Univ.

Keywords

1. Tobermorite
2. Mechanical properties
3. Ab initio molecular dynamics



Mechanical properties of 1.1nm tobermorite using ab initio molecular dynamics

Concrete is widely used as a construction material, and calcium silicate hydrate (C-S-H), which is produced through the hydration reaction between cement and water, is one of its principal constituents. Because C-S-H is largely amorphous and forms through complex chemical reactions, many aspects of its mechanical properties remain unclear. Recent studies, however, have suggested that crystalline tobermorite (specifically 1.1nm tobermorite) formed within C-S-H contributes to the mechanical behavior of concrete, leading to increasing research attention on this phase.

In this context, when considering concrete subjected to fatigue, it is crucial to understand in detail the mechanical properties of C-S-H and 1.1nm tobermorite after they have once experienced compressive loading.

Therefore, in this study, we employed first-principles molecular dynamics to analyze, at the atomic scale, how the mechanical properties change due to stress history by comparing two conditions of 1.1nm tobermorite: initial tension (IT) and tension applied after an initial compression and subsequent unloading (CT). The seminar will present and discuss these results.

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