

博 士 論 文 公 聴 会

ご 案 内

下記の要領で博士論文公聴会を開催します。皆様のご来聴をお待ちしております。

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日 時 : 2024年8月1日(木) 13:30~15:00

場 所 : F608号室

発表者 : Zhuyuan Lin

宇宙地球科学専攻

大阪大学大学院理学研究科宇宙地球科学専攻 後期課程

題 目 : Rheology and Structure of Model Smectite Clay Using
Molecular Dynamics

(分子動力学法を用いたスメクタイト粘土モデルのレオロ
ジーと構造)

宇宙地球科学専攻 大学院教育教務委員

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学位申請者：Zhuyuan Lin

論文題目：Rheology and Structure of Model Smectite Clay Using Molecular Dynamics (分子動力学法を用いたスメクタイト粘土モデルのレオロジーと構造)

論文要旨：

Smectite clay is commonly found in the shallow part of the upper crust and plays a critical role in controlling the rheology and stability of clay-rich faults. Given smectite clay's ability to carry charge and absorb water, conventional understanding based on friction at contact surface may not fully explain its shear resistance. In this study, we perform shear simulations on a model clay system using molecular dynamics, where clay platelets are simplified as oblate ellipsoids interacting via the Gay-Berne potential. The primary aim is to investigate the effect of different factors on the rheology and structure of the model clay system, focusing on strain rate, normal stress and energy anisotropy.

The 3D clay system shows velocity-strengthening behavior with shear dominated by shear bands at low strain rates. The system's structure can be quantitatively described by nematic order and parallel radial distribution function. The shear process at low strain rates in simulation is consistent with experimental observations.

In a 2D clay system under high normal stress, similar structure and rheology to the 3D system are observed. Higher energy anisotropy enhances shear resistance but also promotes cluster formation. The confined 2D system exhibited stick-slip motion together with global velocity-strengthening behavior. Increasing normal stress result in decreasing stress drop. Wall slip near the upper plate is observed at low normal stress and the shear zone is wider at higher normal stress.

Our results suggest the typical characteristics of clay gouge, including velocity strengthening behavior and fabric development during shear, can be observed in this simple model clay system. The shear behavior of clay can be described using a yield stress fluid model beyond conventional considerations on sliding friction. The model clay system can exhibit instability including shear band and stick-slip motion at low strain rate and during shear startup.