

Molecular dynamics study on plastic deformation of silica and silicate materials

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Materials simulations based on classical, first-principles, and machine-learning molecular dynamics methods are considered as a powerful tool for investigating the microscopic atomistic mechanisms of the structural transformation of solid materials, and are applied in a wide range of fields. In the presentation, we will show our several molecular dynamics studies on the plastic deformation behaviors of silica and silicate materials under tensile strain [1], high-pressure [2], shock compression [3], and shear strain and will discuss application of those methodologies to Earth science.

References:

[1] M. Misawa *et al.*, *Sci. Adv.* **3**, e1602339 (2017).

[2] M. Misawa and F. Shimojo, *Phys. Status Solidi B-Basic Solid State Phys.* **257**, 2000173 (2020).

[3] M. Misawa *et al.*, *J. Phys. Chem. Lett.* **11** 4536-4541 (2020).

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