Mineral equilibria in the presence of non-hydrostatic stresses

Moulas E., Geosciences
Speck T., Condensed Matter Physics
Kaus B., Geosciences

Natural minerals occur in a variety of environments, which are commonly characterized by pressure, temperature and chemical composition. In contrast to fluids, minerals (and solids in general) are able to support a significant amount of non-hydrostatic stress. The energetic contribution of non-hydrostatic stress can be such that the classic treatment of using the Gibbs-free energy is strictly-speaking invalid[1].

Over the recent years, molecular dynamic simulations have provided new insights to the importance of non-hydrostatic stress in solids (Fig. 1)[2,3]. However, these studies did not consider geological materials (minerals) and therefore the impact of non-hydrostatic stress on the stability and the phase transitions of minerals remains largely unexplored. Given the wide range of possible stress-states in the earth's crust, the influence of stresses on the phase equilibria is largely unknown.

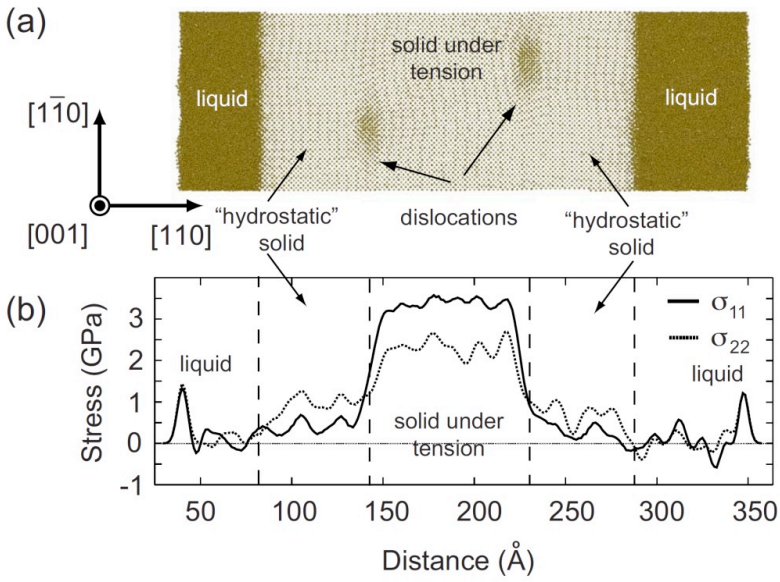

Figure 1. (a) Snapshot of the simulation block during crystallization at T=1271 K. (b) Profiles of the lateral components of stress σ_{11} and σ_{22} across the simulation block. Before the crystallization, the stresses in the solid were σ_{11}=3.4 GPa and σ_{22}=2.3 GPa. Image taken from [2].

The aim of this project is the development of molecular dynamics models that can be used to quantify the mechanical effects on phase transformations in minerals. For that reason, simple and well-characterized mineral phases will be chosen and their phase transformation will be investigated over a broad range of boundary conditions. The results of this study will provide a necessary milestone in the earth-science community where phase transitions always occur in the presence of non-hydrostatic stress.

References

1. Sekerka, R. F. & Cahn, J. W. Solid–liquid equilibrium for non-hydrostatic stress. *Acta Materialia* **52**, 1663–1668 (2004).

2. Frolov, T. & Mishin, Y. Effect of nonhydrostatic stresses on solid-fluid equilibrium. I. Bulk thermodynamics. *Phys. Rev. B* **82**, 174113 (2010).

3. Frolov, T. & Mishin, Y. Effect of nonhydrostatic stresses on solid-fluid equilibrium. II. Interface thermodynamics. *Phys. Rev. B* **82**, 174114 (2010).