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The influence of non-hydrostatic stress on mineral equilibria: insights from Molecular Dynamics

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Mountain building, earthquake generation, and volcanic eruptions occur in Earth's lithosphere and have direct impacts on society. Understanding the mechanism of geodynamic processes relies on the determination of the pressure-temperature history which is recorded by rocks that have been involved in geodynamic processes. In most cases, the interpretation of the conditions attained by rocks is based on the assumption that the stresses in the Earth are hydrostatic. However, non-hydrostatic stresses are observed in the lithosphere, and the significance of the magnitude of the differential stress on phase equilibria is still actively contested among researchers who hold completely incompatible views about the use of various thermodynamic potentials (e.g. [1-3]).

The problem of phase equilibria under non-hydrostatic stress has been explored in several rock-deformation experiments (on mm scale), in which recrystallization of minerals was observed under an applied non-hydrostatic stress [4-6]. However, during experiments, stress and pressure heterogeneities may develop in the sample (e.g. [6]). Therefore, the direct effect of the applied non-hydrostatic stress on the thermodynamics of the reactions cannot be separated from the effect caused by local pressure variations in the sample itself.

Here, we explore the effect of non-hydrostatic stress on the thermodynamics of mineral reactions by investigating a system at the molecular scale. With Molecular Dynamics (MD) we perform coexistence simulations in which two phases are brought in contact and equilibrated at given temperature, pressure, and stress conditions. As expected, the obtained stress component normal to the phase-phase interfaces is homogeneous across the system. Our data suggest that the direct effect of non-hydrostatic stress on the solid-liquid equilibria is rather minor for geological applications, consistent with theoretical predictions [7,8]. However, our analysis does not take into account the indirect effect of stress heterogeneities at the sample scale. Spatial variations of stress can reach GPa level and can therefore indirectly affect phase equilibria.

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