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Precipitation in fluid-mineral systems under differential stress investigated through molecular dynamics

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The interpretation of mineral equilibria and reactions in rocks assumes uniform hydrostatic pressure across all phases. However, such condition is typically not satisfied in geological systems that are composed of multiple phases that are in contact with one another. Stress gradients and non-hydrostatic stresses are to be expected in rocks in the lithosphere, even in the presence of fluids. This complexity challenges the reliability of existing hydrostatic thermodynamic models, and, currently, there is still no accepted theory for evaluating the thermodynamic effect of non-hydrostatic stress on reactions [e.g. 1, 2, 3, 4].

Molecular dynamics (MD) allows us to investigate first-order phase transitions in solid-liquid systems under stress, without the a-priori assumption of a specific thermodynamic potential [5]. With MD simulations the energy of the system, the pressure of the fluid, the stress of the solid, as well as the overall melting and crystallization process can be monitored until the stressed system attains the equilibrium conditions. Our findings indicate that under differential stress, the mean stress of the solid deviates progressively from the pressure of the fluid with which it is in equilibrium. At low differential stresses, deviations from the reference hydrostatic equilibrium are small, allowing accurate phase equilibria predictions by considering the fluid pressure as a proxy for equilibration pressure, as suggested by previous experimental investigations [6].

In the presence of substantial non-hydrostatic stresses, equilibrium between solid and fluid occurs at a fluid pressure significantly higher than hydrostatic thermodynamics predicts. However, the stressed system becomes unstable and a rim of a quasi-hydrostatically stressed solid eventually crystallizes around the initial highly stressed solid core. During the crystallization, the total stress balance is preserved until the newly formed solid-solid-fluid system reaches again a stable equilibrium. At the final equilibrium conditions only the low-stressed solid is exposed to the fluid, bringing back the equilibrium fluid pressure close to the value expected for the equilibrium at homogeneous hydrostatic conditions. Therefore, our results suggest that models describing equilibria and reactions in minerals and rocks under stress can assume that phase equilibria are accurately predicted by using the fluid pressure as a proxy of the equilibration pressure.

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