Si-in-rutile Barometer for Ultra High Pressure Rocks

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The occurrence of Si-rich rutile (18 mol % of SiO_2) in a chromitite body within the ultra-high-pressure metamorphic sequence of Yarlunzangbu ophiolite in Southern Tibet (Yang et al. 2003) suggests that under certain conditions rutile forms a solid solution with stishovite. This opens the possibility of using the stishovite-coesite equilibrium for estimating pressures of crystallization of rocks containing coesite and rutile, since rutile can be treated as stishovite diluted with TiO_2. In this study, the rutile-coesite equilibrium is calculated as a function of pressure and temperature using the tabulated thermodynamic properties of coesite and stishovite (Holland and Powell, 1998) and a model for the activity of stishovite in the stishovite-rutile solid solution, which is evaluated herein. The thermodynamic mixing properties of the SiO_2-TiO_2 solid solution were modelled based on first principles calculations of the formation energies of supercell structures of rutile and stishovite with single (Si or Ti) and paired (SiSi or TiTi) defects inserted at all possible distances within the supercell. These energies were converted to the pair interaction constants, which were combined to get an approximation for the excess enthalpy of any Si/Ti configuration in the solid solution. The temperature-dependent enthalpy and the Gibbs free energy of mixing were calculated using Monte Carlo simulations. Our results suggest that the free energy in the stishovite-rutile join is strongly asymmetric, such that the mixing is possible only at the rutile side. At 10 GPa and 2000 K, rutile equilibrated with coesite dissolves about 2 mole % of SiO_2. This prediction is in good agreement with the experimental data of Ren et al. (2005).

References

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