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Interaction between water and point defects inside volume-constrained α-quartz: An ab initio molecular dynamics study at 300 K

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Quartz-based minerals in earth's crust are well-known to contain water-related defects within their volume-constrained lattice, and they are responsible for strength-loss [1-3]. Experimental observations of natural α-quartz indicate that such defects appear as hydroxyl groups attached to Si atoms, called Griggs defect (Si-OH), and molecular water (H2O) located at the interstitial sites. However, factors contributing to the formation of Griggs and interstitial H2O defects remain unclear. For example, the role of point defects like vacancy sites (O2- and Si4+), and substitutional (Al3+) and interstitial (Li1+, K1+, Ca2+, Mg2+, etc.) ions has remained largely unexplored. Here, we performed ab initio molecular dynamics at 300 K to examine the energetics and structure of water-related defects in volume-constrained α-quartz. Several configurations were systematically interrogated by incorporating interstitial H2O, O2 and Si4+ vacancies, substitutional Al3+, and interstitial Li1+, Ca2+ and Mg2+ ions within α-quartz. Interstitial H2O defect was found to be energetically favorable in the presence of Substitutional Al3+, and interstitial Ca2+, Mg2+, and Li1+. In the presence of O2- and Si4+ vacancies, H2O showed a strong tendency to dissociate into OH—to form Griggs defect—and a proton; even in the presence of substitutional and interstitial ions. These ions distorted the α-quartz lattice and, in the extreme case, disrupted long-range order to form local amorphous domains; consistent with experimental reports. Our study provides an initial framework for understanding the impact of water within the crystal lattice of an anhydrous silicate mineral such as quartz. We provide not only thermodynamic and process-related information on observed defects, but also provides guidelines for future studies of water's impact on the behavior of silicate minerals. Our findings are published in the Journal of Applied Physics: https://doi.org/10.1063/5.0190356.

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