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Development of a Robust Procedure for Generating Structural Models of Calcium Aluminosilicate Glass Surfaces

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Abstract : The structure-property relationships of calcium aluminosilicate (CAS) glass surfaces are of scientific and technological interest regarding dissolution phenomena. Molecular dynamics (MD) simulations can provide atomic-scale insights into the structure and properties of the CAS interfaces in vacuo as the first step to conducting computational dissolution studies on CAS surfaces. However, one limitation to date is that although the bulk properties of CAS glasses have been well studied by MD simulation, corresponding efforts on CAS surface properties are relatively few in number (both theoretical and experimental). Here, a systematic computational protocol to create CAS surfaces in vacuo is developed by evaluating the sensitivity of the resultant surface structure with respect to different factors. Factors such as the relative thickness of the surface layer, the relative thickness of the bulk region, the cooling rate, and the annealing schedule (time and temperature) are explored. Structural features such as ring size distribution, defect concentrations (five-coordinated aluminium (AlV), non-bridging oxygen (NBO), and tri-cluster oxygen (TBO)), and linkage distribution are identified as significant features in dissolution studies.

Keywords : MD simulation, CAS glasses, surface structure, structure-property, CAS interface
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