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Assessing the transferability of ReaxFF for alumina polymorphs

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ABSTRACT

The objective of this study is to assess the transferability of the ReaxFF interatomic potential for alumina polymorphs using energy calculations and virtual diffraction characterization. This study includes simulations of bulk, surface, and interface alumina structures containing the ?-, ?-, ?-, and a-Al_2O_3 phases. Transferability of the ReaxFF interatomic potential is determined by comparing computed bulk, surface, and interface energies to prior experimental and simulation results. In addition, minimum energy structures are characterized using a virtual diffraction method that generates experimentally comparable X-ray diffraction and electron diffraction patterns. Analysis of these results identifies a key limitation of the ReaxFF interatomic potential for alumina that biases formation of an amorphous phase. Although data show ReaxFF correctly predicts the energetic stability of a-Al_2O_3 among the bulk crystalline alumina phases, it incorrectly predicts an even lower energy amorphous phase. Experimental comparison of the virtual X-ray diffraction patterns constructed for each bulk phase validates the minimum energy bulk crystalline structures. However, virtual selected area electron diffraction patterns of alumina surface models show significant surface reconstructions at temperature due to the energetic bias for amorphization. Discrete peaks within these virtual diffraction patterns show that complete amorphization of the surfaces does not occur due to the constraints imposed by the interior atoms.