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Investigation of the (Pt,Pd)BiTe and (Pt,Pd)Te2 bulk and surface stability at 300K using AIMD-MLFF

This study adopted the ab-initio molecular dynamics (AIMD) modelling technique imbed-ded within the Vienna ab-initio simulation package (VASP). The machine learned force field (MLFF) was utilized for robustness of the AIMD simulations. These methods were adopted unravel the bulk and surface stability of the platinum group minerals (PGMs) such as moncheite (PtTe2), merenskyte (PdTe2), michenerite (PdBiTe) and maslovite (PtBiTe) minerals at room temperature (300 K). The AIMD-MLFF trained bulk models produced lattice parameters of: a = b = 4.026 Å, c = 5.221 Å for PtTe2, a = b = 4.040 Å, c = 5.133 Å for PdTe2, a = b = c = 6.746 Å for PtBiTe, a = b = c = 6.749 Å for PdBiTe. The generated force field applied on the 4x4x4 supercells. The 4x4x4 supercells produced lattice parameters of: a = b = 4.079 Å, c = 5.283 Å for PtTe2, a = b = 3.982 Å, c = 5.130 Å for PdTe2, a = b = c = 6.716 Å for PtBiTe, a = b = c = 6.719 Å for PdBiTe These were in agreement with the experimental lattice parameter a = b = 4.049 Å, c = 5.288 Å for PtTe2, a = b = 3.978 Å, c = 5.125 Å for PdTe2, a = b = c = 6.689 Å for PtBiTe, a = b = c = 6.646 Å for PdBiTe.
The (001) surface for (Pt,Pd)Te2 and (100) surface for (Pt,Pd)BiTe were determined to be the most stable surfaces from computed X-ray diffraction (XRD). The ab-initio surface energies were calculated as 0.42 J/m2 for PtTe2 and 0.31 J/m2 for PdTe2. For (Pt,Pd)BiTe the surface energies were 0.75 J/m2 for PtBiTe and 0.78 J/m2 for PdBiTe. The AIMD-MLFF surface ener-gies correlated with those from ab-initio simulation where by the surface energies of 0.73 J/m2, 0.80 J/m2, 0.44 J/m2 and 0.33 J/m2 were obtained for PtBiTe, PdBiTe, PtTe2 and PdTe2, respec-tively. These showed that the (Pt,Pd)Te2 minerals have lower surface energies than the (Pt,Pd)BiTe minerals, suggesting that the former cleaves easily compared to the latter. These showed that the AIMD-MLFF method is a feasible method for simulation of minerals.

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