Friction of Alumina Borate from Molecular Dynamics Simulations: A Lubricant for Space Exploration

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Alumina borate, formulated as $10Al_2O_3 \cdot 2(B_2O_3)$, emerges as a promising solid lubricant for space exploration due to its remarkable hardness and reduced coefficient of friction (COF). Within this study, we explored the lubricating dynamics of boron trioxide (B_2O_3)—a glass-forming compound known for its friction-minimizing properties when it transitions into a glassy layer. Utilizing ReaxFF molecular dynamics (MD) simulations, we examined how COF evolves with various velocities and temperatures. The simulation setup involved a dual-layer coating of B_2O_3 on both upper and lower Al_2O_3 substrates, with alumina borate inserted between them as a lubricant. To accurately simulate chemical reactions, we employed recently developed Al/B/O ReaxFF parameters. Moving velocities from 0.1 m/s to 20 m/s were applied to the upper substrate, with temperature ranges from 300K to 1500K. Contrary to initial expectations that higher velocities and temperatures would increase COF, our findings reveal that COF initially rises before diminishing across these variables. Notably, specific combinations of velocities and temperatures were identified as critical factors contributing to elevated COF levels.

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