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ENHANCING MECHANOCHEMICAL SODIUM BOROHYDRIDE REGENERATION THROUGH PROCESS OPTIMIZATION AND ENERGY DISSIPATION MODELING

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High-energy ball milling presents a promising pathway for the sustainable regeneration of sodium borohydride ($NaBH_4$), a potent hydrogen storage medium. In this work, we integrate experimental process optimization with predictive energy dissipation modeling to advance mechanochemical regeneration techniques. Experimentally, a systematic investigation of key operational parameters—milling time, ball-to-powder ratio, molar ratio, and rotational speed—reveals that prolonged milling and the careful balance between ball-to-powder and reactant ratios are pivotal for achieving high conversion yields [1].

Complementarily, discrete element method simulations are employed to study the mechanics of ball milling by quantifying normal and tangential energy dissipation. Master curves developed from these simulations enable the prediction of energy transfer under untested operational conditions, highlighting the roles of fill ratio, ball size, and rotational speed in determining process efficiency. By correlating energy dissipation profiles with experimental yield data, our integrated approach provides a robust framework for optimizing both the mechanochemical process and the design of milling equipment. This synergy between experimental insights and simulation-driven predictions paves the way for more efficient and scalable hydrogen storage technologies.

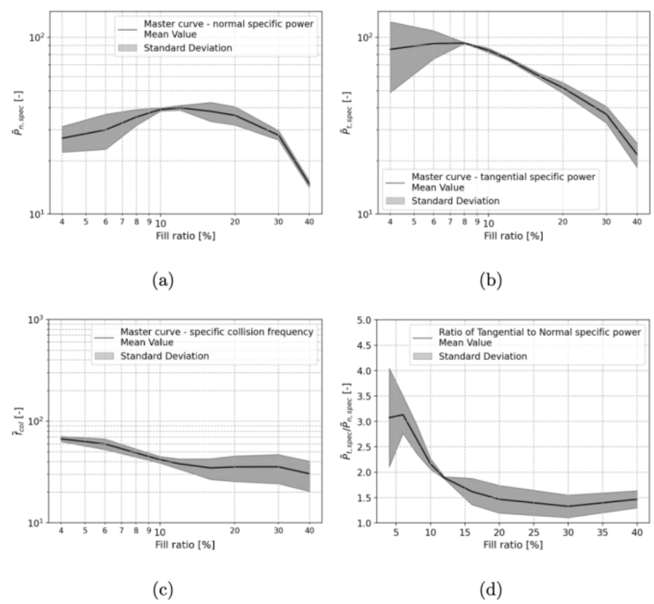

Figure 1. a) Master curve - mean specific normal power dissipation per collision. b) Master curve - mean specific tangential power dissipation per collision. c) Master curve - mean specific collision frequency. d) Ratio between mean specific tangential power dissipation per collision and mean specific normal power dissipation per collision. Calibrated coefficients (system comprising ($NaBO_2 \cdot 4H_2O$) and (MgH_2)).

[1] Garrido Nuñez, S.; Schott, D. L.; Padding, J. T. Int. J. Hydrogen Energy **2025**, 97, 640–648