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Garrido Nuñez, S.; Schott, D.L.; Padding, J.T.

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ABSTRACTS

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EFFECT OF TANGENTIAL-TO-NORMAL STRESS DISTRIBUTION ON THE MECHANOCHEMICAL REGENERATION OF $NaBH_4$

Santiago GARRIDO[a], Dingena SCHOTT[b], Johan PADDING[a]

[a] *Department of Process & Energy, TU Delft, Delft, The Netherlands*
[b] *Department of Maritime & Transport Technology, TU Delft, Delft, The Netherlands*

s.garridonunez@tudelft.nl

Although mechanochemistry is maturing as a solvent-free synthesis route, the distinct roles of shear-dominated (tangential) and compression-dominated (normal) stresses inside ball mills remain largely unquantified. Recent analyses point out that most mechanochemical models still collapse the full stress tensor into a single scalar “pressure”, leaving the influence of stress anisotropy “surprisingly unexplored”[1]. Insight has begun to emerge from tribological model systems, such as ZDDP tribofilm formation, where shear and normal stresses can be varied independently, but these tests do not replicate the collision statistics of a ball mill and therefore cannot gauge their impact on practical solid-state synthesis [2]. Here we supply an unbiased reactor-scale comparison of tangential- and normal-dominated regimes for the practical solid-state synthesis of NaBH4.

Discrete element method (DEM) mechanical descriptors were leveraged to design experiments with matched constant-speed and constant-power to decouple total power input from the distribution of tangential and normal stressing events in the mechanochemical regeneration of NaBH4. A low fill ratio (6 %), which maximizes tangential dissipation, achieved a record 94% regeneration yield while reducing the ball to powder ratio by 40%, shortening milling time by 38 %, and reducing milling speed by 34% compared to previous literature results.

The specific yield (product per Watt) peaked at 0.28 yield/W, and yield declined linearly with fill ratio ($R^2 > 0.99$); increasing the fill level from 6% to 17% reduced conversion by 40%–50% without any energy benefits (Fig. 1). Because the key DEM descriptors $\{E_n, E_t, f_{col}/n_{ball}\}$ are mill-agnostic, the results provide a transferable blueprint for energy-efficient scale-up and cross-platform benchmarking.

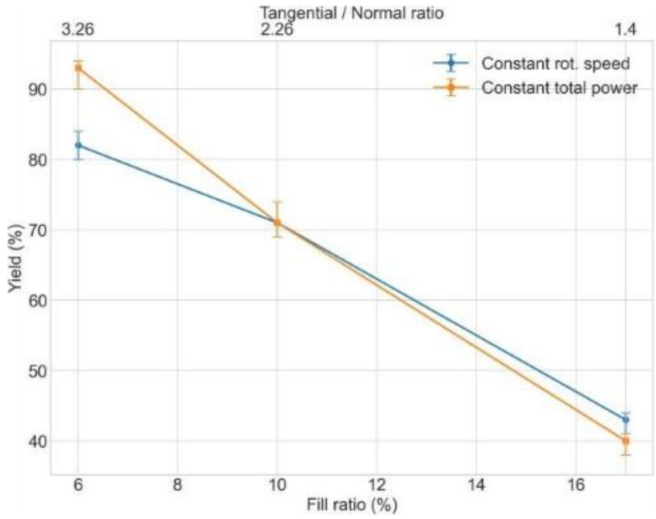

Figure 1. Yield versus fill ratio for experiments run (i) at constant rotational speed (blue) and (ii) at constant total power (orange). The secondary (top) axis converts each fill ratio to the corresponding tangential/normal dissipation ratio inside the jar. Error bars show the variability in yield.

[1] Sergey V. Sukhomlinov, Guido Kickelbick, Martin H. Müser, *Tribol. Lett.* **2022**, *70*, 102.
[2] Lu Fang, Spyridon Korres, William A. Lamberti, Martin N. Webster, Robert W. Carpick, *Faraday Discuss.* **2023**, *241*, 394-412.