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Supporting information

Collision model methodology for the calculation of energy in planetary ball mill

To simplify the calculation of energy in the planetary ball mill, the following assumptions are made [11]:

- The balls and the interval wall of the vial are covered with a thin layer of powder, as this allows all the kinetic energy to be transferred to the powder particles from the ball impact.
- The energy is only generated from the collisions between balls and the wall the balls move against the opposite wall without rolling and sliding

The total energy transferred to the planetary ball mill P^* normalised to the powder weight (PW) as a function of time t is shown in Equation S1 [11], [12] ;

$$P^* = \frac{Pt}{KPW} = -\varphi_b N_b m_b t (W_p - W_v) \left[W_v^3 \frac{\left(R_v - \left(\frac{d_b}{2}\right)\right)}{W_p} + W_p W_v R_p \right] \frac{\left(R_v - \left(\frac{d_b}{2}\right)\right)}{2\pi PW} \quad \text{Equation S1}$$

Where P is the total power of the system, φ_b , ε and η_v correspond to the geometrical parameters related to the number of the balls, and the vial's dimensions, N_b is the number of balls, m_b is mass of ball, W_p is the angular velocity of the plate, W_v is the absolute angular velocity of the vial, R_v is the distance from the centre of the vial to its periphery, R_p is the distance from the centre of the mill to the centre of the vial and d_b is the ball diameter. φ_b can be derived using Equation S2,

$$\varphi_b = (1 - \eta_v^\varepsilon) \quad \text{Equation S2}$$

where ε can be calculated using Equation S3 with $N_{b,v}$ and $N_{b,s}$ and expressed according to Equation S4 and Equation S5 respectively. $\varphi_b = (1 - \eta_v^\varepsilon)$ are geometrical parameters associated with the number of balls in the vial which depict the degree of filling of the vial.

$$\varepsilon = \log(0.05) / \log\left(\frac{N_{b,v}}{N_{b,s}}\right) \quad \text{Equation S3}$$

Where, $N_{b,v}$ represents the number of balls that can arrange in a simple cubic manner to fill the vial with the diameter D_v , as shown in Equation S4 [19].

$$N_{b,v} = \pi D_v^2 H_v / 4 d_b^3 \quad \text{Equation S4}$$

Where, $N_{b,s}$ represents the number of balls that can arrange in a simple cubic manner to cover one-third of the inner surface of the wall which is calculated according to Equation S5 [19].

$$N_{b,s} = \pi (D_v - d_b) H_v / 3 d_b^2 \quad \text{Equation S5}$$

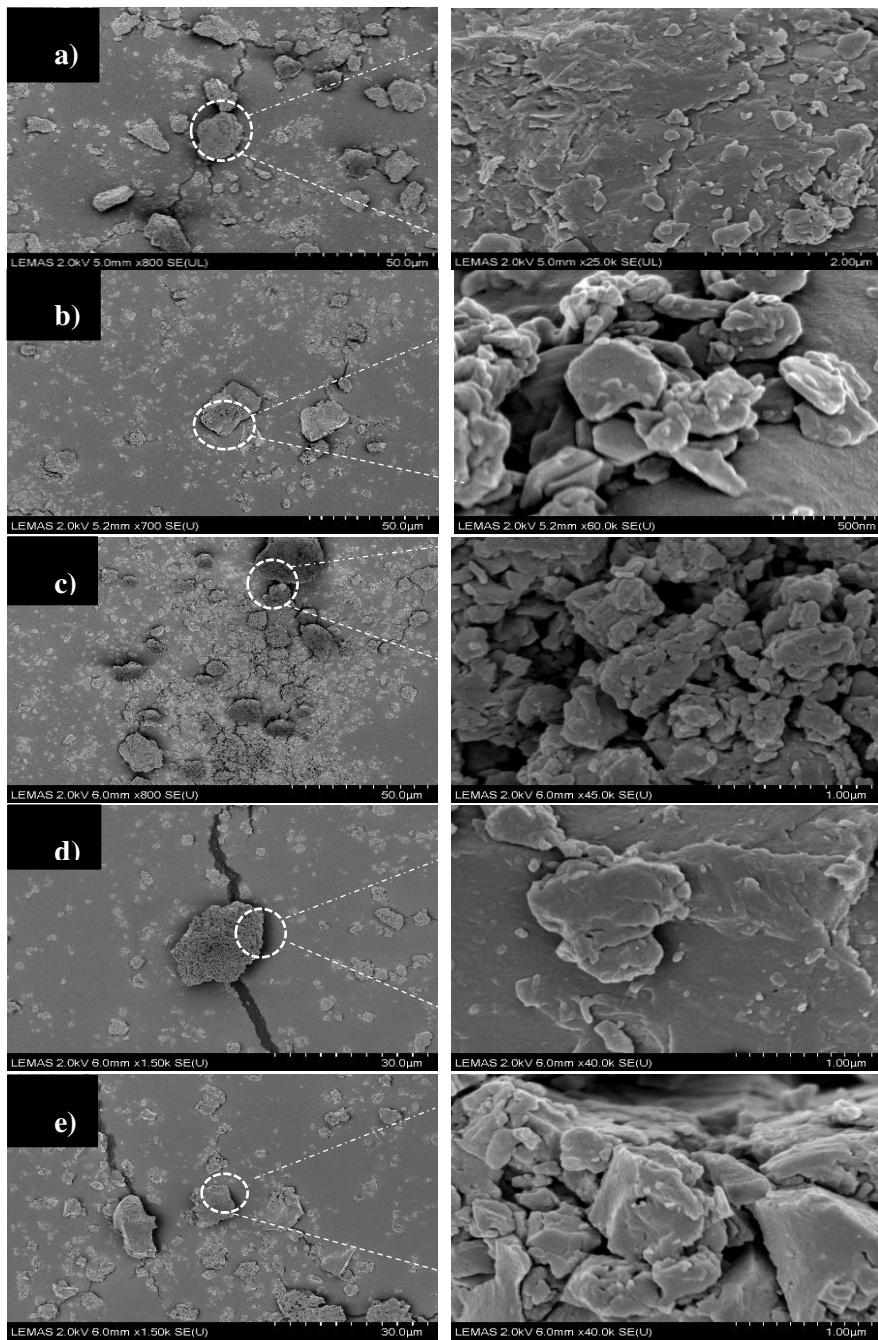


Figure S1: SEM images show the Morphology of DABOMD particles (left) and their surfaces (on the right), a) Non-milled, b) 1min milled, c) 5min milled, d) 15min milled, e) 300min Single Ball Mill.

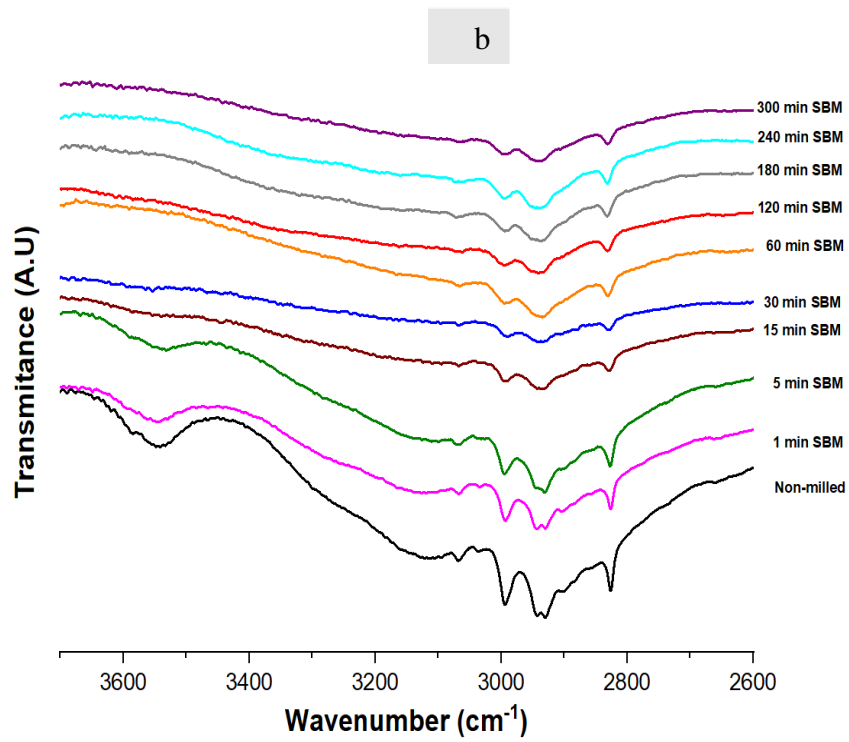
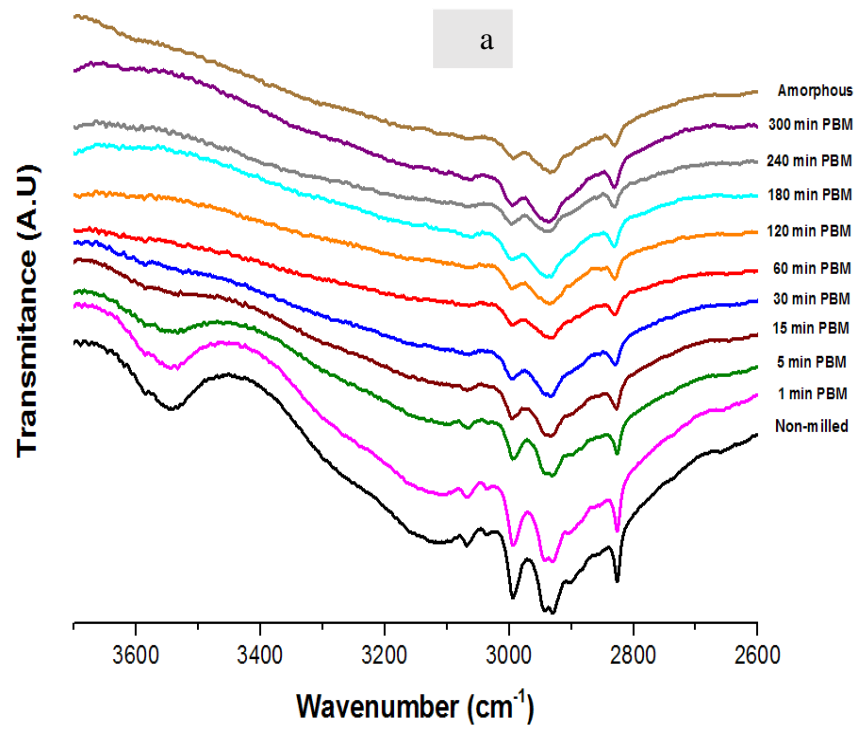


Figure S2: FTIR-ATR of non-milled and milled DABOMD showing scan from 2600 to 3700 cm^{-1} . a) Planetary ball milled (PBM) (Reproduced with the permission of American Chemical Society (ACS) [1]. b) Single ball milled (SBM)