Article:
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Table 1: Planetary ball mill variables

Milling Variables	Symbol	Value
Number of balls	N_b	4
Powder weight (kg)	PW	0.0125
Angular velocity of the plate (rad.s^{-1})	W_P	68.07
Milling time (s)	t	60-1800

Table 2: Planetary ball mill geometrical parameters

Geometrical variable	Symbol	Value
Diameter of the ball (m)	d_b	0.02
Weight of the ball (kg)	m_b	0.032
Diameter of the pot (m)	D_v	0.12
Height of the pot (m)	H_v	0.106
Distances from the centre of the mill to the centre of the vial (m)	R_p	0.12
Distances from centre of the vial and the centre of the vial to its periphery (m)	R_v	0.06
Absolute angular velocity of the vial rad s−1	W_v	136.1

Table 3: Single ball mill variables

Milling Variables	Symbol	Value
Diameter of the ball (m)	d_b	0.015
Weight of the ball (kg)	m_b	0.014
Powder weight (g)	PW	1.3
Coefficient of restitution	CoR	0.16
Milling vessel dimensions		
Length (mm)	Diameter (mm)	Half sphere (mm)
38	9	9

Table 4: DEM simulation parameters for PBM

Planetary ball mill	PM100
Pot material	Steel
Pot material density ρ (gcm-3)	7.8
Shear modulus (GPa)	210
Poisson Ratio	0.25
Coefficient of restitution of the powder-steel	0.16
Powder-powder sliding friction coefficient	1.53
Powder-Steel sliding friction	0.73
Rolling friction	0.01
Simulation time t (sec)	6
Simulation time step (sec)	2.0×10^{-6}

Table 5: DEM simulation parameters for SBM

Single ball mill	MM200
Pot Material	Steel
Shear Modulus (GPa)	210
Poisson's Ratio	0.25
Density (gcm-3)	7.8
Particle original diameter ($\boldsymbol{um}$)	21.2
Scale-up particle diameter ($\boldsymbol{um}$)	232.3
Shear modulus of powder (Pa)	10^8
Density of the particle ($\boldsymbol{Kg/m^3}$)	1500
Coefficient of restitution of the powder-steel	0.16
Powder-powder sliding friction coefficient	1.53
Powder-Steel sliding friction	0.73
Rolling friction	0.01
Simulation time t (sec)	4
Simulation time step (sec)	2.8×10^{-7}

Table 6: Characteristic sizes (D_{10}, D_{50}, and, D_{90}) of non-milled and milled DABOMD in planetary ball milled (PBM) ((Reproduced with the permission of American Chemical Society (ACS) [18] and in single ball milled (SBM)

Sample	Particle Size (μm)			Sample	Particle Size (μm)		
	D_{10}	D_{50}	D_{90}		D_{10}	D_{50}	D_{90}
Non-milled	1.5	21.2	211	Non-milled	1.5	21.2	211
1 min PBM	1.5	16.4	186	1 min SBM	1.4	13.7	171
5 min PBM	1.7	12.7	98.1	5 min SBM	1.7	11	76.8
15 min PBM	1.7	11.2	66.9	15 min SBM	1	6.1	51.1
30 min PBM	1.7	9.9	58.9	30 min SBM	1.2	7.6	52
60 min PBM	1.7	9.9	51.8	60 min SBM	1.4	8.4	58.9
120 min PBM	1.6	8.7	45.6	120 min SBM	1	6.8	45.6
180 min PBM	1.7	8.7	40.1	180 min SBM	0.7	5	45.7
300 min PBM	1.5	7.5	35.3	300 min SBM	1	6.1	48.2

Table 7: Percentage Water content from TGA of samples milled with planetary ball mill and single ball mill

Time (min)	Water content from TGA PBM (%)	Water content from TGA SBM (%)

1	8.7	8.7
5	8.3	8.4
15	7.7	8.3
30	7.2	8.0
60	6.5	7.3
120	5.9	6.6
180	5.3	5.7
300	4.7	5.0

Table 8: Vibrations of the main functional groups in non-milled crystalline and milled DABOMD in planetary and single ball mills

Functional group	Type of vibration mode	Crystalline vibration (cm^{-1})	Amorphous vibration (cm^{-1})	300 min PBM vibration (cm^{-1})	300 min SBM vibration (cm^{-1})
O-H	Stretch	3300-3600	3070-3660	3070-3660	3070-3660
S=O	Stretch	1001.2	993.9	994.9	996.0
C-H in CH3 or O-CH3	Stretch	2929.5	2934.1	2935.7	2939.7
Benzimidazole H3C-O	Bend	1197.7	1197.8	1198.1	1198.6

Table 9: Table shows the outcome of the model fit of the kinetics of comminution amorphisation in planetary ball mill and single ball mill

Parameters	Comminution Kinetics		Amorphisation Kinetics		Dehydration Kinetics	
	PBM D90	SBM D90	PBM (XRPD)	SBM (XRPD)	PBM	SBM

k_1	0.28	0.4	0.2	0.17	0.190	0.160
k_2	0.01	0.04	0.02	0.01	0.019	0.010
α	81%	88%	81%	76%	15%	12%
τ_{rpd}	3.6	2.5	5.3	5.9	5.3	6.3
τ_{slw}	88.3	25	52.3	100	52.6	100

Table 10: Energies for PBM, SBM and Compression test

Calculated Energyin PBM following Collison model	The total power of PBM P (J/s)	253.2
	The total power of PBM P (J/g.s)	20.3
Experimental Energy in SBM following high speed camera	Impact energy SBM E_b (J/g) Mill power (J/g.s)	0.028 1.68
Energies from Compression Test	Compression energy (J/g)	5.52

Energy from DEM in simulation PBM	Collision power in PBM (J/g.s)	9.33
Energy from DEM simulation SBM	Impact power in SBM (J/g.s)	3.42

Table 11: shows the amount of energies used to generate different size, and amount of amorphous in planetary ball mill and single ball mill

DABOMD	PBM Energy Transferred to the System				SBM Energy Transferred to the System			
Time (min)	D90 (μm)	AAC (%)	Collison Model calculation (kJ/g)	DEM simulation (kJ/g)	D90 (μm)	AAC (%)	High-speed camera tracking (kJ/g)	DEM Simulation (kJ/g)

0	211	0	0	0	211	0	0	0
1	186	37.8	1.22	0.56	171	29.1	0.10	0.21
5	98.1	55.7	6.09	2.80	76.8	53	0.50	1.03
15	66.9	77.8	18.27	8.40	51.1	62.4	1.51	3.08
30	58.9	88.1	36.54	16.79	52	76.7	3.02	6.16
60	51.8	93.1	73.08	33.59	58.9	85.2	6.05	12.31
120	45.6	95.6	146.16	67.18	45.6	93	12.10	24.62
180	40.1	97	219.24	100.76	45.7	93.1	18.14	36.94
240	_	97.7	292.32	134.35	-	95.3	24.19	49.25
300	35.3	98.2	365.40	167.94	48.2	96	30.24	61.56