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Feature article

Modeling of the planetary ball-milling process: The case study of ceramic powders

M. Broseghini [a], L. Gelisio [a], M. D'Incau [a,*], C.L. Azanza Ricardo [a], N.M. Pugno [b,c,d], P. Scardi [a]

[a] Department of Civil, Environmental & Mechanical Engineering, University of Trento, via Mesiano, 77, 38123 Trento, Italy
[b] Department of Civil, Environmental & Mechanical Engineering, Laboratory of Bio-Inspired and Graphene Nanomechanics, University of Trento, via Mesiano, 77, 38123 Trento, Italy
[c] Center for Materials and Microsystems, Fondazione Bruno Kessler, Via Sommarive 18, 38123 Povo (Trento), Italy
[d] School of Engineering and Materials Science, Queen Mary University of London, Mile End Road, London E1 4NS, United Kingdom

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ABSTRACT

A numerical dynamic-mechanical model of a planetary ball-mill is developed to study the dependence of process efficiency on milling parameters like ball size and number, jar geometry and velocity of the revolving parts. Simulations provide evidence of the correlation between milling parameters and the resulting microstructure of the ground material. In particular, maximum efficiency of the grinding process is observed with the most disordered ball motion, which is obtained within a well-defined range of jar to plate velocity ratios. As a significant case study in ceramic powder technology, the model is presented and validated for calcium fluoride (CaF_2), ground under different conditions in a planetary mill, and then characterized by X-ray powder diffraction and scanning electron microscopy.

1. Introduction

High-energy ball milling is commonly used for particle size reduction (comminution) down to the nanometer scale [6,16,62]. Increased surface energy and defectivity lead to modified physical/chemical properties and can promote structural transformations and/or chemical reactions (see *e.g.* [67]). Nearly all materials can be processed, including metals [12,50,59], organics [31,54,61] and pharmaceuticals [39,47,48], as well as composites [14,40] or low-dimensional structures [2,8,15,38,71]. Ceramic materials can be produced either (i) indirectly or (ii) directly [58] *via* ball milling. While the former route promotes enhanced reactivity of starting materials (due to morphological, structural and/or chemical modifications) [34] and/or their deagglomeration [50], therefore improving the consecutive thermal treatment, the latter results in the direct manufacture of the desired end-product [10,35,60,68]. This is usually nanostructured, characterized by a selected polymorph [19,69,70], and affected by defects which are exploited to tune selected properties [24,29]. Furthermore, ceramics can be incorporated into different matrices by ball milling, so to enhance mechanical properties [28].

Among high-energy ball mills, the planetary is a mechanically simple and versatile device for efficient grinding. It is usually made of two or more jars, rotating at an angular velocity ω around their axis (see Fig. 1), installed on a disk rotating at angular velocity Ω. Grinding occurs by impact among the milling media (balls and jars), driven by centrifugal and Coriolis forces, with material particles typically covering balls and/or jar surfaces. The energy available for comminution and, in turn, the size of the ground particles and their defectivity, are determined by several parameters, related both to geometry and to physical properties of jar and milling media. These include size and shape of balls and jar, elasto-plastic properties and friction coefficients, but also angular velocities, grinding time and charge fraction. Products homogeneity and contamination from the vials are also related to the above-defined parameters and must be properly accounted for. The (i) straightforward approach to correlate milling parameters to end products is running the mill under different conditions. The alternative to this brute-force, time consuming empirical approach is modeling the process, either (ii) analytically [1,5,51] or (iii) numerically [17,30,33,42,44,53]. The main advantage of modeling over experimental testing is a better control over kinematic and dynamic quantities, *e.g.* ball trajectories and kinetic energies, under all possible operating conditions. Analytical models are elegant and informative but, most often, limited by simplifying assumptions, like inelasticity of collisions or approximate friction models. Numerical multibody models, although more

* Corresponding author.
E-mail address: mirco.dincau@unitn.it (M. D'Incau).

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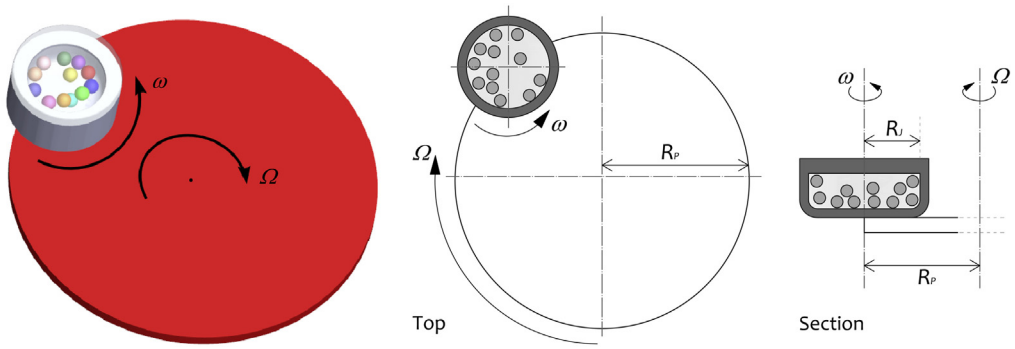

Fig. 1. Schematic representation of a planetary ball-mill. Left, three-dimensional view; middle and right, definition of the jar radius R_j and the distance between axis of rotation (angular velocity ω) and revolution (angular velocity Ω) R_p.

computationally demanding, can preserve the main complexity of the milling process and possibly provide more accurate predictions.

This work introduces a model belonging to the latter category, implemented within the framework of a multibody dynamics software. The validity of the model has been experimentally verified considering the case study of a typical ceramic material, calcium fluoride.

2. The model

Following, the model of the Fritsch Pulverisette 4 (P4 [18]) planetary ball mill is presented. The solution of the equation of motion of the milling media is obtained, implementing a suitable model for contacts and Lagrangian description, by the software MSC.Adams [45]. One of the most appealing features of this multibody dynamics software is the aptitude for handling complicated mechanical systems, therefore allowing a detailed description of different processing apparatuses. Due to its limited volume fraction, powder charge has not been explicitly modeled but accounted for by a suitable choice of collision contact parameters [17], as will be discussed later.

The Hilber–Hughes–Taylor (HHT [26,46]) integrator, with automatic step tuning, was adopted setting a maximum numerical error of 10^{-8}.

2.1. The mill

The angular velocities ω and Ω (see Fig. 1) were applied, respectively, to the two hinges (features predefined in the MSC.Adams software) connecting (i) the jar (radius R_J) to the main disk (radius R_P = 125 mm) and (ii) the latter to the ground reference frame. Milling media were randomly placed inside the jar, in the gravitational field, and angular velocities were gradually increased to the target values during the first second of simulation, which lasted overall 24 s. To allow motion homogenization, the first 4 s were discarded during data analysis. Properties of jar and milling media are reported in Table 1.

2.2. Contact modeling

The most critical ingredient in the model of a ball mill is the contact law.

Contact models belong either to the (i) discrete or (ii) continuous approach [20]. While (i) is based on momentum balances, in (ii) a force–displacement law is added to the equation of motion, as a combination of a spring in parallel with a damper, causing energy dissipation, plus a friction element. The most significant formulations are based on a combination of either linear or non-linear spring or damper but more complicated schemes, such as those based on Mindlin's work or on the introduction of plasticity, have also been proposed [13,20,22,37,53].

Table 1
Geometrical and physical properties of jar and milling media for the presented case study.

Jar (AISI 304)	
Radius	32.5 mm
Volume	80 cm^3
Density	8.03 g/cm^3
Young modulus	193 GPa
Poisson ratio	0.29

Spheres (AISI C1020)	
Number	12
Radius	6 mm
Density	7.85 g/cm^3
Young modulus	200 GPa
Poisson ratio	0.29

The contact force is defined by the hard-coded *impact function* [45], based on the non-linear spring (F_k) and linear damper scheme (F_d) proposed by Dubowsky and Freudenstein (impact pair model [13]),

$$F_c = F_k + F_d = ku^n + c\dot{u}, \tag{1}$$

being u and $\dot{u}$ the relative displacement and velocity of the colliding bodies, whereas k and c are the spring generalized stiffness and the damping coefficient. With respect to the above formulation, to prevent discontinuities, the *impact function*, defined within MSC.Adams, implements a damping coefficient which depends on the relative displacement of colliding bodies,

$$c = -c_m \left(\frac{u}{d}\right)^2 \left(3 - 2\frac{u}{d}\right), \tag{2}$$

and varies from zero to c_m, assuming the latter value when the relative displacement is greater than or equal to d. With the exponent n = 3/2, an estimate of k can be derived from the Hertzian theory of contact [22],

$$k = \frac{4}{3\pi}\left(\frac{1}{\eta_i + \eta_j}\right)\sqrt{\frac{R_i R_j}{R_i + R_j}}, \tag{3}$$

for the contact between sphere i and j, with radius R, and

$$k = \frac{4}{3\pi}\left(\frac{1}{\eta_i + \eta_j}\right)\sqrt{R_i}, \tag{4}$$

for the contact between sphere i and a plane (approximating jar surface). The parameter $\eta_i = (1 - \nu_i^2)/(\pi E_i)$ accounts for elastic properties of materials, being ν the Poisson ratio and E the Young modulus. The solution of the classical problem of damped vibration