Discrete element simulation of the dynamics of high energy planetary ball milling processes

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Abstract

This paper outlines a discrete element based numerical simulation framework for the investigation of some dynamic aspects of planetary ball milling processes. The general principles of the discrete element approach is briefly presented, followed by the discussion of several particular computational issues related to the simulation of planetary ball mills. A numerical example is presented to demonstrate the applicability of the procedure developed.

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1. Introduction

High energy ball milling processes, including attrition mills, SPEX shaker mills and planetary ball mills, have been established as a non-equilibrium mechanical processing technique to achieve solid state amorphisation of various alloy systems and nano-crystalline materials [1–4]. Due to this significant scientific and industrial importance, considerable research [5–7] has been conducted on the modelling of mechanical alloying processes, mainly based on mechanical and thermodynamic approaches, to predict the physical characteristics and microstructure of the milled powders. Most models are established on the basis of the assumption of several dynamic features of the ball milling process, and in particular, the patterns of impact velocity/energy and impact frequencies. The dynamics of ball milling processes is largely determined by such operation conditions as the number and size and the physical properties (density, surface hardening, etc.) of the milling balls; properties and characteristics of the metal powder; ball/powder weight and volume ratio; shape, dimensions and material of vials and milling velocities, etc. Thus, gain of a reasonable level of understanding of the ball milling dynamics can provide a better insight into the basic mechanisms associated with high energy ball milling processing for the formation of amorphous phases, which consequently may lead to the improvement of existing designs, and to the optimisation of the milling conditions for a particular milling case.

However, the dynamic process of high energy ball milling, particularly planetary ball milling, is still far from fully understood. The difficulty is mainly associated with the complex physical phenomena involved in the process characterised by highly dynamic, non-linear behaviour of a multi-physics and multi-scale nature. This difficulty, together with a considerable number of controllable operation parameters and their combinations, makes any attempt to investigate such process experimentally almost intractable, if not impossible. Some effort has been made in the development of mathematical models to study the dynamics of various high energy ball milling processes and some comprehensive surveys can be found in [8,9]. Nevertheless, most approaches may be considered preliminary since some assumptions made may significantly oversimplify the real situations. The present work aims to provide a discrete element based numerical simulation framework for the investigation of the dynamic aspects of planetary ball milling processes. Early work on the topic can be found in [10].

2. Discrete element approach

The discrete element method (DEM) [11,12] is a numerical approach for the analysis of systems with discrete/
discontinuous features. It is similar to molecular dynamics (MD) in the concept that individual material elements are considered and represented separately, but different in that the shape of each individual object need not be the same, and in the ways that the objects interact with each other. The major building blocks for the DEM are briefly described below.

2.1. Discrete element representation

In the DEM, not only disks in 2D and spheres in 3D can be employed to represent simple shaped discrete bodies, but other geometric entities such as points, segments/facets, ellipses/ellipsoids, and polygone/polyhedra can also be used. In addition, discrete objects with more complex geometric shapes are often represented by the cluster/clumping of simpler geometric entities, or may be specially designed for particular cases, as will be shown later.

2.2. Contact/interaction detection

The DEM assumes that discrete bodies are (possibly) connected only along their boundaries by appropriate physically based interaction laws, with short-ranged mechanical contact being the main contact response. The most important algorithmic aspect of the DEM is to determine the actual interaction forces among discrete objects. This interaction contact detection comprises three phases: (global) spatial search, (local) interaction resolution and interaction force computation.

In the first phase, different shaped objects are approximated by simple geometric entities such as disks/spheres or rectangles that bound the objects concerned. By examining their relative spatial locations, any potential contact/interaction pairs among discrete objects are detected. It is essential to employ highly effective contact search algorithms in this phase, particularly when a large number of bodies are present in the system.

In the second phase, each potentially contacting pair identified in the previous global search is locally resolved based on their actual geometric shapes, and pairs without interaction are excluded.

Following the local interaction resolution, the interaction forces between each actual interaction pair are determined from a constitutive relationship or physical interaction law. In this paper, contact interaction laws have been employed within the framework of penalty methods. The penalty method only approximately satisfies the contact displacement constraints for finite values of the penalty coefficients, allowing a small amount of overlap to occur in (local) small contact regions. In general, the interaction laws describe the relationship between the overlap and the corresponding repulsive force between a contact pair. The Hertz contact model that governs elastic contact of two spheres is adopted here as the normal contact model. Energy dissipation due to plastic deformation, heat loss and material damping, etc. during impact is taken into account by adding a viscous damping term into the model.

2.3. Solution of the dynamic equation systems

The dynamics of discrete element systems is governed by Newton’s second law. The resultant forces for each discrete element include contact interaction forces, external applied forces such as gravity and any additional (global) damping forces specified. The evolution of the whole system can be determined by solving the dynamic equations numerically. Due to the high speed dynamic impact nature of the problem, the governing equations of the system are solved by explicit time integration schemes and the central difference algorithm is employed in this work. The explicit time integration scheme generally imposes a constraint on the maximum time step to be applied. This condition, together with the consideration of solution accuracy, requires the use of a very small time step (often \( < 10^{-6} \) s), resulting in a substantially large number (usually in excess of one million) of time steps having to be performed.

3. Simulation issues of planetary ball milling

When applying the above discrete element procedure to planetary ball mills, several issues need to be discussed further. Fig. 1 illustrates a schematic diagram of a planetary ball mill.

Fig. 1. A schematic diagram of a planetary ball mill (cross-section).
The motion of the vial is predetermined in terms of each component. The vial is not a simple geometric entity, it is represented by a compound object consisting of a top and bottom disk, a cylinder and a quarter of a torus. Each component is a primitive geometric entity and can be described analytically. Also, the contact detection between the vial and balls can be decomposed into the contact between balls and wall which may exhibit some randomness. Consequently, the modified interaction laws should also possess such random features. It is however not easy to establish such a mathematical model as many factors may contribute to the phenomenon.

A possible solution to the problem is to conduct a local modelling, as shown in Fig. 2, by employing the same discrete simulation approach. This small scale model comprises two impacting balls (or one ball and a wall) and some powder particles. The presence of the particles represents the powder trapped between the balls/wall. By varying the number or density of the packed powder particles around the balls/wall, the arrangement patterns, impact conditions (such as impact velocity and angle) then different impact characteristics of the balls/wall can be simulated. The subsequent analysis of the results obtained may lead to a statistical impact model which can be used as the interaction laws in the global simulation.

The current work adopts the third option but the randomness of the interaction laws is not fully taken into account. More specifically, the previously mentioned effects of powder on ball impact are considered in the model by using a lower (nominal) Young’s modulus of both milling balls and vial and larger damping ratios. In addition, larger friction coefficients (for both sliding and rolling) are assigned, and the values are assumed to vary randomly within a range.

4. Numerical illustration

The numerical procedure outlined in the previous sections will be demonstrated for the simulation of a planetary ball milling process. Since some parameters used may differ from a real situation, the results obtained are mainly for illustrative purposes.

The following geometric and operational parameters are chosen: $L = 125\, \text{mm}$, $R_g = 40\, \text{mm}$, $R_c = 15\, \text{mm}$, $H =$...
Fig. 3. Number of normal impacts vs. time.

Fig. 4. Impact percentages in different velocity bands.

60 mm, \( \omega_g = 300 \text{ rpm} \), \( \omega_l = -2.5 \omega_g = -750 \text{ rpm} \). The radius \( r_b \) and the mass density \( \rho \) of the milling balls are respectively 5 mm and 7860 kg/m\(^3\). The nominal Young’s modulus \( E \) for balls and vial is set to be \( 10^9 \text{ Pa} \), and the impact damping ratio \( \xi \) is 0.5. The sliding friction coefficient \( \mu_s \) is in the range of \([0.2, 0.5]\) and the rolling friction coefficient \( \mu_r \) is taken as half of the sliding value. Simulations are conducted with the number of milling balls being 10 and 20, respectively. The milling balls are originally deposited arbitrarily within the vial.

Since the Hertz model with an additional viscous damping term is employed as the normal contact model, with the values of \( r_b, \rho, E \) and \( \xi \) given above, the impact force and duration are determined by the initial normal impact velocity. For an impact velocity of \( v_n = 4 \text{ m/s} \), the maximum impact force is around 2000 N and the impact lasts for about 5 \( \mu \text{s} \). Based on this observation, the time step is taken as \( 5 \times 10^{-7} \text{ s} \), which is sufficiently small to satisfy the stability requirement for the central difference scheme.

5. Concluding remarks

The current work has outlined a discrete element based numerical strategy for the simulation of the dynamics of planetary ball milling processes. The proposed approach possesses several advantages over other analytically based modelling procedures. The most important features are that each impact could be stimulated and the effects of any change of operation conditions on the dynamics of the system can be easily investigated. The present work however is regarded as a preliminary study, and further work on several aspects needs to be pursued. For instance, experiments should be undertaken to validate the results, and also to provide the required parameter values in the model. Actual ball milling is a much longer and time consuming process, which may take several hours to several days, whereas the DEM procedure, with current computer capacities, can simulate the process only up to tens of seconds within a reasonable CPU time scale, which is far too short. In addition, the milling conditions undergo constant changes during the process as a result of severe plastic deformation, thermal effects, and even chemical reactions of the milled powder. It is not straightforward however to incorporate all these dynamic changes in physical characteristics of the metal powder into the current model. Thus, some integration with other numerical/mathematical modelling procedures may be essential in order to achieve a more complete understanding of high energy ball milling dynamics.

References