Chemical Engineering Science 101 (2013) 366–373

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

Discrete element model for an attritor mill with impeller responding to interactions with milling balls

Priya R. Santhanam, Alexandre Ermoline, Edward L. Dreizin *

New Jersey Institute of Technology, Newark, NJ 07102, United States

HIGHLIGHTS

- Energy dissipation by the milling tools is accurately predicted for an attritor mill.
- The accuracy is achieved by a DEM description accounting for interactions of the moving impeller and the milling balls.
- The interaction is quantified using time-resolved torque and rotation rate measurements.
- The new model predicts energy dissipation rates for different materials.
- The model enables an accurate assessment of the milling dose required for the manufacturing scale-up.

ARTICLE INFO

Article history:
Received 26 March 2013
Received in revised form
21 June 2013
Accepted 26 June 2013
Available online 5 July 2013

Keywords:
Particle processing
Scale-up
Mechanical alloying
Ball milling
Powder technology
Simulation

ABSTRACT

This work advances discrete element modeling (DEM) as a tool for predicting milling progress for mechanical alloying, reactive milling, and similar mechanical milling-based techniques for material preparation and modification. DEM is used to predict the rate of energy dissipation by the milling tools, which is correlated with the milling progress. The model is considered for attritor mills, which are most likely to be used in industrial settings. In attritor mills, milling balls may jam causing an increased resistance to the impeller's rotation. The impeller may, therefore, instantaneously slow down, quickly returning to its pre-set rotation rate. Previous DEM models did not account for such rapid changes in the impeller's rotation rate, which caused gross errors in the predicted rates of energy dissipation. Experiments using a laboratory mill established a correlation between the impeller's torque and instantaneous rotation rate. This correlation was programmed in a DEM model, where changes in the rotation rate could occur because of the impeller's interaction with milling balls. Predicted energy dissipation rates were shown to correlate well with the experimental data. A modified DEM approach enables one to accurately predict milling conditions for different scale attritor mills necessary for manufacturing advanced materials.

1. Introduction

Ball milling is a versatile and scalable technique for processing and preparation of a wide range of materials, including advanced mechanically alloyed powders (Suryanarayana, 2008; Zhang, 2004), powder-like components of energetic materials (Ren et al., 2010; Umbrajkar et al., 2008; van der Heijden and Leeuwenburgh, 2009), materials for energy storage (Aguey-Zinsou et al., 2007; Hanada et al., 2005; Liang et al., 1999), structural applications in aircraft, automotive and military industries (Mohammad Sharifi et al., 2011), etc. The range of potential applications for mechanical milling as a materials processing technology is rapidly expanding, including preparation of solid dosage forms in pharmaceutical industry (Lefort et al., 2004), battery components (Machida et al., 2005; Raphaël Janot, 2005), materials for food processing (Liu et al., 2011), artificial bone compositions (Mohammadi Zahrani and Fathi, 2009), and remediation of contaminated soil (Montinaro et al., 2007). Despite discovery of many advanced materials that could be prepared by milling, practical and commercial manufacture of such materials poses significant challenges. In particular, it is difficult to predict which milling conditions should be used in a practically scaled milling device to reproduce an advanced material prepared in laboratory experiments. Such predictions should rely on a validated theoretical description of material refinement, suitable to describe milling devices of different types and scales.

Discrete element modeling (DEM) is well suited and has been used extensively to describe operation of various ball mills,

* Corresponding author. Tel.: +1 973 596 5751.
E-mail address: dreizin@njit.edu (E.L. Dreizin).

0009-2509/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.ces.2013.06.048

e.g. (Cleary, 1998; Jayasundara et al., 2008; Kwan et al., 2005; Mishra, 2003; Mori et al., 2004; Zhu et al., 2008). DEM used in the modeling and simulation of tumbling mills has been successful in producing excellent prediction of (net) power consumption, liner and media wear and mill output (tonnage and size distribution). However, with respect to the application of the DEM methodology to mechanical alloying performance, direct comparisons between the DEM-predicted characteristics and experimental results are not straightforward. One common denominator for both experimental and computational data is the energy transferred from milling tools to the powder being milled. Respectively, an energy-based parameter, milling dose, was introduced as a useful concept in our previous work (Jiang et al., 2009; Santhanam and Dreizin, 2012, 2013; Ward et al., 2005). The milling dose, D_m, is defined as the energy transferred from milling tools to the powder, normalized by the powder mass, m_p:

$$D_m = \frac{E_d}{m_p} t \tag{1}$$

where E_d is the rate of energy dissipation from milling tools and t is the milling duration. It was suggested that the same material could be prepared in different milling devices if the same starting powders were used and if the same milling dose was transferred to the material from milling tools. The successful application of this approach depends on how accurately the milling dose is predicted by DEM descriptions for different milling devices. For example, if a material of interest is prepared in a small scale shaker mill, the D_m value can be obtained using the experimental milling time, t_{exp}, and a DEM model quantifying the energy dissipation rate by milling balls in the shaker mill, E_d. This milling dose can now be used to predict the milling time required to prepare the same material in a different mill, using DEM to appropriately calculate the respective energy dissipation rate.

The concept of milling dose was explored comparing material preparation in a shaker, planetary, and attritor mills (Santhanam and Dreizin, 2012, 2013). The first two mills are common in laboratory experiments; the attritor is more suited for commercial scale manufacture. Theoretical models of the milling devices were set-up to obtain the respective E_d terms. In experiments, the same material was prepared using the same starting powders in each mill. Respective milling times, t, and mass loads, m_p, were recorded. The milling dose values for the shaker and planetary mills were close to each other, as expected. However, the computed energy dissipation rate for the attritor was very high, resulting in a much greater than expected milling dose. It was noted that in the attritor mill computation, balls were often predicted to jam, resulting in unrealistically strong forces exerted onto the milling media from the impeller moving at a constant, pre-set speed. These predicted high-force interaction events result in a substantially over-predicted rate of energy dissipation, making the respective DEM description inadequate.

In experiments, ball jams can also occur; however, they cause small changes in the impeller speed. Thus, the variations in the force are attenuated. Santhanam and Dreizin (2012, 2013) proposed a screening scheme to account for the computationally predicted events associated with unrealistically high forces, in which any events involving unrealistically high forces were discarded. The resulting, corrected milling dose for the attritor was much closer to that predicted for other milling devices.

Although that approach was effective to obtain the desired outcome, a DEM description that represents the actual operation more directly, without superficial screening, is desired and developed here. The model enables instantaneous changes in the rotation speed of the impeller responding to instantaneous changes in the resistance caused by the milling balls. Recent results on experimental monitoring of rotation rate and torque in the attritor mill (Santhanam and Dreizin, 2012, 2013) as well as additional experiments are used to tune the developed model. The predictions of the developed model are discussed in terms of both accuracy of the assessed energy dissipation and its use for evaluation of the milling dose.

2. Materials and methods

2.1. Experimental

Detailed descriptions of the milling conditions, materials and characterization techniques can be found elsewhere (Santhanam and Dreizin, 2012, 2013), and they are only briefly outlined here. An oxide dispersion strengthened aluminum–magnesium oxide (Al•MgO) composite was prepared in three different mills, including an attritor, shaker and planetary, in order to assess and compare the milling dose required to prepare the same material in different devices. The same starting materials, pure aluminum (−325 mesh, 99.9% pure, by Atlantic Equipment Engineers) and magnesium oxide (−325 mesh, 99% pure, by Aldrich Chemical Company, Inc.) blended at 70%/30% Al/MgO volume ratio were used. The same 9.5-mm diameter hardened steel milling balls were used in all three mills.

In each mill, the milling balls became coated with the powder and thickness of the formed coating was assessed experimentally. First, mass of uncoated balls was recorded, and then the balls coated with the powder were recovered after selected milling times and weighed. The results of these measurements are shown in Table 1 in terms of the average weight of the powder coating on one milling ball and its standard deviation from measurements taken at different milling times. The mass shown in Table 1 is affected by both pre-set ball to powder mass ratio and dynamics of ball motion in each mill.

Yield strength of consolidated powders served as an indicator of the milling progress and was measured as a function of milling time for the powders prepared in each mill.

The present model focuses on experiments using an attritor mill, model 01HD by Union Process. In this mill, milling balls are agitated by a steel impeller rotating at a designated speed. In the experiments, the impeller was set to rotate at 400 rpm. The attritor mill contains a built-in data acquisition unit by Baldor. It was used to measure the torque and rotation speed as a function of milling time (Santhanam and Dreizin, 2012, 2013). The mechanical power required to turn the impeller was calculated from the product of torque and the rotation speed. The data were collected at different milling times; each collected data set was recorded for 1 s with a time resolution of 1 ms.

In order to explore the effect of powder properties on the energy dissipation rate, in addition to experiments with Al•MgO composites, experiments were also performed with a powder blend of Al and B_4C (70/30% by volume) and with sand.

In experiments (Santhanam and Dreizin, 2012, 2013), the attritor vial filled with the steel milling balls contained 1.8 kg of balls and 50 g of powder. Additional experiments were performed, in which the torque and rotation rate were measured for reduced loads. Specifically, balls were loaded with their masses

Table 1
Average mass of powder coating per milling ball for different mills.

Milling device	Ball to powder mass ratio	Mass of powder coating per milling ball, g
Shaker mill	10	0.010 ± 0.009
Planetary mill	3	0.019 ± 0.011
Attritor mill	36	0.007 ± 0.005