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A system dynamics model to estimate energy, temperature, and particle size in planetary ball milling

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Abstract

System Dynamics (SD) is a mathematical method of modeling to understand and analyze complex problems. In this study, assuming collision as the dominant energy transfer event, a SD model was for the first time developed to quantify milling energy in planetary ball mills. The main advantage of this modeling approach is that the dependency of various milling parameters is considered. The milling energy estimated by the SD model, which is derived from Majini-Iassona equations, allows predicting the mean particle size and milling temperature as a function of time. A good agreement was found between the results of the model and some experimental studies, suggesting the merit of the proposed model.

Keywords: Powder metallurgy; Microstructure; Kinetics

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1. Introduction

Ball milling as a powder processing technique has several applications in metallurgy and ceramic industries. The final microstructure strongly depends on the energy of the milling process. Despite widespread studies conducted to simulate various aspects of milling, a comprehensive model to quantify milling energy is essential to be developed. This model allows predicting the evolution of temperature and powder particle size vs. milling time.

Ball milling involves several features to achieve the preferred product phase, microstructure, and properties [1], complicating the process modeling. Because of this compiexity, the dependency of some parameters has been ignored in previous studies. Typically, Benjamin and Volin [2] conducted the early research to estimate the particle size as a function of the milling time during the 1970s. Another study was to predict the temperature rise during collision between two balls and the powder [3]. Also, Maurice and Courtney [4] reported two studies on geometry, mechanics, and physics of ball milling. The most important groups that conducted some systematic researches on modeling of the milling process include Maurice and Courtney [5], Gaffet et. al [6], Magini and Iasonna [7], Koch [8], and Watanabe el at. [9]. A few others have also focused on the representation of the mechanism of this production method [10].

In this study, to consider the dependency of these milling features, for the first time, the System Dynamics (SD) programming method was used. SD is a mathematical method of modeling to understand and analyze complex problems in industries. Jay Forrester developed this method in the 1950s, to help corporate managers to improve their understanding of industrial processes [11]. Although it is possible to perform the SD modeling in a spreadsheet, there are various software packages optimized for the SD modeling. In this

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research, the software package used to analyze the milling energy was Vensim PLE written and distributed by Ventana group [11].

2. Methodology

Essentially, for the milling process, the variables affecting the milling energy can be classified into two groups: powder and process parameters. The main powder parameters include the atomic mass, powder density, and heat capacity of initial mixed powder. One the other hand, the milling container volume, milling time, milling speed, grinding medium size, ball-to-powder weight ratio, and extent of vial filling are the process features [12].

In the case of the powder parameters, a comprehensive Microsoft Access database of elemental physical properties was collected and linked to the SD model. Afterwards, incorporating the atomic number and fraction of each element as the input data called from the database, the physical properties of powders were estimated using the linear rule of mixtures. With regard to the process variables, the extent of vial filling, ball-to-powder weight ratio, elasticity of collision, and ball velocity are dependent [13]. Considering milling time as the main independent variable, the others are restricted according to Table 1.

SD programming is typically composed of conceptual model, causal loop diagram, and calculations, to analyze the dependency of various involving parameters, as detailed below.

2.1. Conceptual model

The primary stage of the SD model development of the planetary milling process is conceptualization. To design a conceptual model, the purpose of the model, the model boundary, the shape of the reference modes, and the nature of the basic mechanisms should be determined [14]. In this way, a novel conceptual model was developed based on the energy conservation law, considering the milling kinetic energy as the main factor.

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During milling, collisions can be either elastic, which causes the particle size reduction and the generation of crystal defects, or inelastic, which increases the process temperature and often releases thermal energy. Schematically, the milling energy per collision can be conceptualized as a box which contains the elastic and inelastic terms and also their consequences (Figure 1).

2.2. Causal loop diagram

The most important feature of this approach is to clarify the intrinsic structure of milling, to see how different parameters relate to others [15]. According to the conceptual model of milling process designed by the authors, a typical causal loop diagram for the SD model was developed (Figure 2).

In this casual loop, the time-dependent milling energy of grinding media is considered as a level variable. This can be consumed by a temperature increase (or thermal energy waste) and/or a particle size decrease (or crystal defects generation) in terms of inelastic and elastic energies, respectively. Incorporating the powder and process parameters, the causal loop estimates the milling temperature and particle size as a function of milling time. Note that in this model, the milling vial was considered to be adiabatically isolated, i.e. the thermal energy waste is eliminated. Additionally, the crystal defects generation as a complicated metallurgical event was ignored. In fact, the complexity of the milling process is conceptually simplified by three different submodels, analyzing the evolution of kinetic energy of ball milling, temperature, and particle size [16]..

2.3. Model calculations

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As mentioned above, there are three submodels in the developed causal loop, the energy generation, the milling temperature increase, and particle size reduction. Therefore, formulating the milling energy model for SD programming without the analysis of these parts is unattainable.

i) Milling energy

Magini and Iasonna [17] suggested a model supposing the collision as the main energy transferring event. Evaluating the kinetic energy of the balls and the amount of material entrapped in the collision event, they derived a useful equation expressing the energy transferred per unit of mass in a planetary mill (Equation 1).

$$\Delta E = Q_{max}\left[7.66x10^{-2}R_p^{1.2}\rho^{0.6}E^{0.4}\right]d_b\omega_p^{1.2}/\sigma \quad (1)$$

where R_p, ρ, E, d_b, ω_p, and σ are introduced as milling plate radius, grinding medium density, elastic modulus, mean diameter of balls, milling speed, and powder surface density, respectively. Also, the maximum quantity of material trapped during each collision, Q_{max} is given by Equation 2.

$$Q_{max} = 2\sigma\pi R_{h,max}^2 \quad (2)$$

where $R_{h,max}$ as the radius of contact at the maximum of compression during each collision is calculated by Equation 3.

$$R_h = 1.1076((V_b^{0.4}m_b^{0.2}R_p^{0.4})/E^{0.2}) \quad (3)$$

Using Equations 1, 2, and 3 proposed by Magini and Iasonna [17], here it is suggested that the energy transferred per unit of mass in each collision can be estimated by Equation 4.

$$\Delta E = 5.904\times10^{-1}R_p^{1.2}\rho^{0.6}d_b\omega_p^{1.2}V_b^{0.8}m_b^{0.4}R_p^{0.8} \quad (4)$$

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ii) Temperature increase

Assuming that, under the given milling conditions, an amorphous phase or a crystalline phase could be formed in the powder, the temperature experienced by the powder would determine the nature of the phases [18].

Firstly, Magini and Iasonna [17] studied the energy transferred to the powders during milling in a planetary ball mill and a SPEX mill. Assuming that the energy results in an adiabatic temperature rise, ΔT can be given by Equation 5, where c is the specific heat of the powder [19].

$$\Delta T = \Delta E / c.Q_{max} \tag{5}$$

From experiments, in the early stages of milling, most of the powder adheres to the surface of the balls and the vial walls. Measuring the weight of the balls as a function of the milling time, the surface density of the powder covering the balls can be estimated. However, in this study, to estimate the value of the powder surface density, it is assumed that a grinding medium is wetted by one layer of the powder. So, the powder surface density as an effective parameter during the milling process can be estimated by Equation 6.

$$\sigma \approx \rho_p d \tag{6}$$

where ρ_p is the powder density and d is the mean diameter of powders. Using Equations 1, 5, and 6, an equation expressing the maximum temperature increase in each collision is proposed as Equation 7.

$$\Delta T_{max} = 7.66\times10^{-2}\left(R_p^{1.2}\rho^{0.6}E^{0.4}d_b\omega_p^{1.2} / \rho_p.d\right) \tag{7}$$

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Using the volume filling factor derived from the ball, powder, and mill container volumes, the "elasticity factor" that considers the elasticity interaction between balls and walls can be calculated. Assuming this factor presented in Ref. [7], the calculated trajectory of the waste thermal inelastic energy becomes more realistic.

iii) The particle size

Although it is impossible to estimate exactly the amount of energy required to reduce the particle size of a given material, several empirical laws have been proposed [20]. Kick calculated the grinding energy according to Equation 8 [21].

$$E = C_K \ln\left(d_0 / d_f\right) \tag{8}$$

where E, C, d_0, and d_f are the grinding work (in kJ/kg), grinding coefficient, particle size of the source material, and particle size of the ground material, respectively. The kick's equation supposes that the energy required is directly related to the reduction ratio. It means that the energy required to crush a given amount of material from 10 mm to 5 mm size is the same as that required to reduce the size from 2 mm to 1 mm.

Since the surface of a unit mass of material is proportional to $1/d$, Rittinger suggested the energy required for the size reduction is directly proportional to the increase in surface (Equation 9) [21].

$$E = C_R \left(\frac{1}{d_f} - \frac{1}{d_0}\right) \tag{9}$$

And Bond proposed Equation 10 to estimate the energy required for the size reduction [21].

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$$E = C_B \left(\frac{1}{\sqrt{d_f}} - \frac{1}{\sqrt{d_0}} \right) \tag{10}$$

Note that experiments show that the Kick's equation is more accurate for coarse particles (d > 50 mm) and the Rittinger's equation is more suitable for fine particles (d < 0.05 mm), while the Bond's equation is proper for the intermediate particle sizes [21].

2.4. Model validity

To evaluate the validity of the proposed model estimating the milling energy and particle size, the SD model result was compared to experimental data of Ref. [13]. The initial powder mixture was Fe(bcc)-17 wt.% C with a particle size of 11 μm. Room-temperature milling was conducted in a planetary ball mill (R_p = 25 cm) with a vial volume of 300 cc at a milling speed of 200 rpm. Tempered steel balls of 10 mm in diameter with a ball-to-powder weight ratio of 10:1 were also used. In addition, to assess the particle size prediction by the model in the fine scale, a powder particle size of 2 μm with the above process conditions was studied.

To describe the temperature evolution during the milling process, the results of the SD model were compared to experimental data. Starting the powder mixture of Fe(bcc)-17 wt.% C with a particle size of 10 μm, room-temperature milling was conducted in a Fritsch P-5 planetary ball mill with an insulated vial volume of 300 cc at a milling speed of 200 rpm. A digital thermometer with the sensitivity of 0.1 K was employed for the determination of powder temperature after every 1 h of milling, similar to Ref [19].

3. Results and discussion

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First, the mathematical model described above was used to estimate planetary ball milling energy. Figure 3 compares the milling energy calculated by the SD model with that calculated via measured milling power, to check the model's validity. The similar linear trend of this parameter vs. milling time and the acceptable compatibility of the experimental data and model results verify the merit of the proposed SD model.

Assuming the adiabatic system, Figure 4 shows the instantaneous temperature variation of the powder determined by the model and experiment. It can be observed that the trend and amount of the temperature determined by the model and experiment are in good agreement. The estimation of the milling temperature could help to guess thermally-activated phase transformations during milling process [22]. Moreover, the milling temperature is one of the most effective factors in the formation of final microstructure [23].

Since the main purpose of the milling process is decreasing powder particle size [24], the prediction of the mean particle size vs. milling time is valuable. Figure 5(a) represents the mean diameter of the milled powder vs. milling time, estimated by the model. According to this figure, the model predicts a decrease in the powder particle size with milling time. Comparing the model results and the experimental data presented in Figure 5(b), it can be realized that the trends observed in the experiment and numerical model are similar, inferring the model validity.

5. Conclusions

In this paper, a SD model was introduced to quantify the milling energy, mean particle size, and milling temperature vs. time in planetary ball mills. The following conclusions can be drawn from this study:

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1. In the analysis of milling energy as a function of time, the model results and experiments showed a similar trend.

2. Supposing an adiabatic insulation system attached to milling tools, the maximum temperature during the milling process vs. time was successfully estimated via the inelastic term of the kinetic energy.

3. The experimental mean particle size as a function of milling time was similar to that predicted by the SD model.

4. As the model quantitatively predicted the trends observed in the experiments, it is suggested that the model can well explain the progress of the milling process.

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Figures

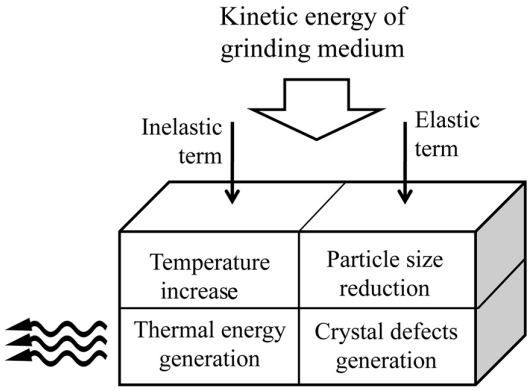

Figure 1. Conceptual model of milling energy applied to the entrapped powder.

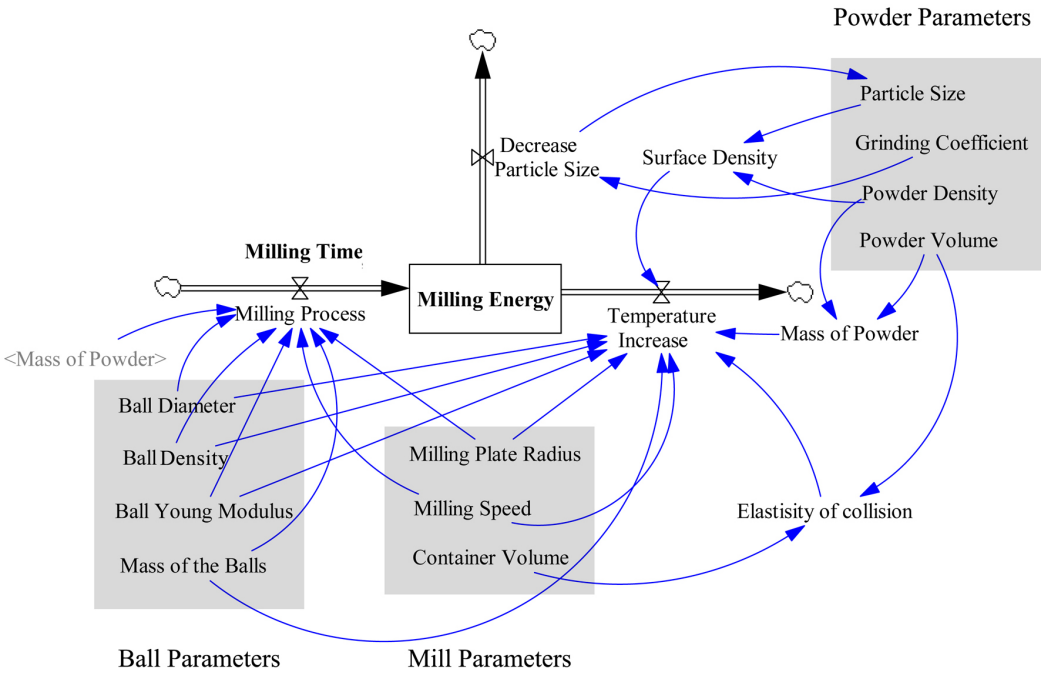

Figure 2. Causal loop diagram for the SD model.

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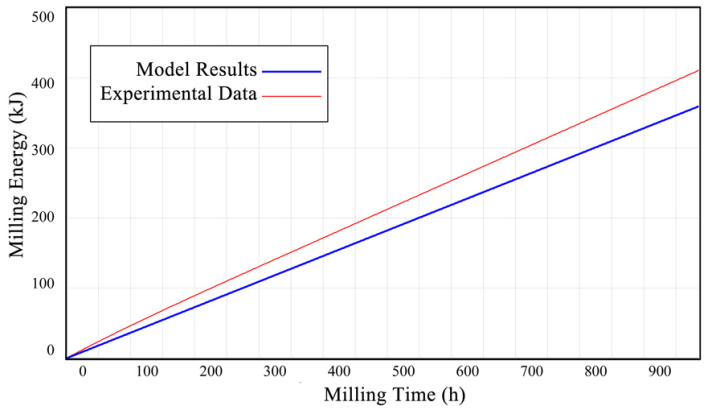

Figure 3. Milling energy determined by the SD model and experiment of Ref. [13].

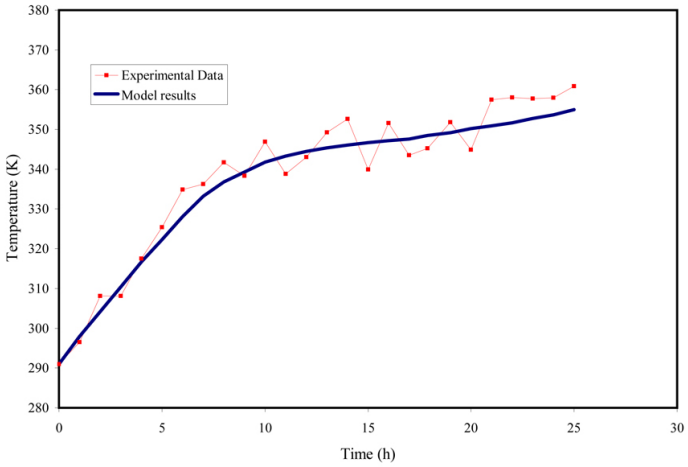

Figure 4. Comparison between the modeled and experimental temperature changes during planetary ball milling.

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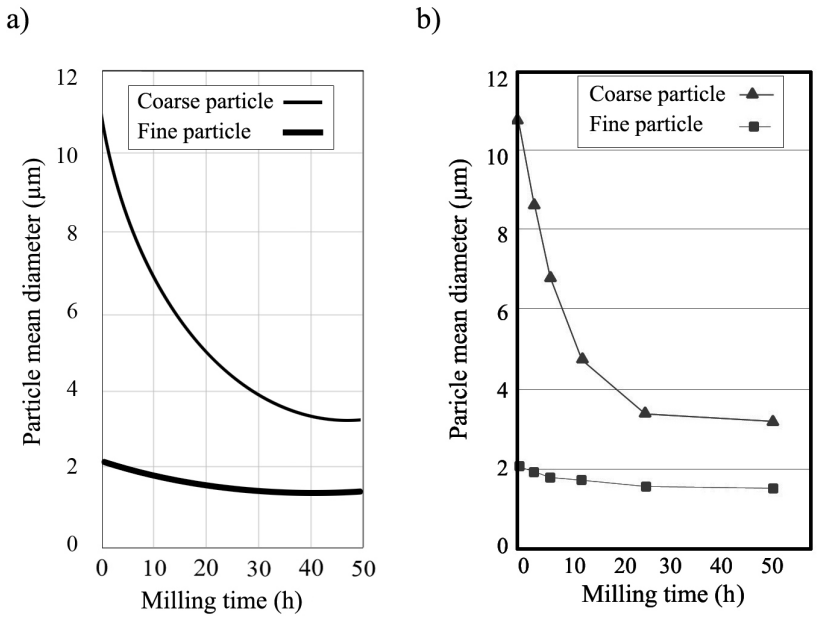

Figure 5. Mean diameter of the milled powder vs. milling time: (a) model results and (b) experimental data reported in Ref. [13].

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Table

Table 1. Minimum and maximum values of process variables in SD modeling.

Variable name	Mill container volume (cc)	Milling speed (rpm)	Mean diameter of balls (m)	Number of balls	Mill plate radius (m)
Min. value	20	50	0.01	10	0.1
Max. value	300	400	0.02	300	0.5