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# Computer Simulation of Mechanoactivation Process in the Planetary Ball Mill: Determination of the Energy Parameters of Milling

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**Abstract** - Analysis of milling process in a planetary ball mill was carried out by computer simulation. A character of a ball motion depending on a vial occupancy was studied. The dependences of energy dissipation and average temperature in a vial on the filled fraction and size of balls are determined. Contributions of tangential and normal collisions of balls to the magnitude of energy dissipation were considered. The values of energy dissipation and temperature for various milling materials were estimated. The results of computer simulation were compared with the calculated results obtained using analytical formula and with literature data as well. The obtained results allow to choose the optimal modes of ball milling with regard to the specific character of concrete problems.

## INTRODUCTION

The interest to mechanical alloying (MA) process was caused by an opportunity of obtaining nonequilibrium phases and nanocrystalline structures which are of both scientific and practical importance.

The result of MA process depends on mill design: geometric and dynamic parameters, character of motion of milling bodies, their physical and mechanical characteristics, as well as those of processed substances, a mass ratio of milling bodies to powder etc. [1 - 8]. A magnitude of energy dissipation was proposed as a general criterion for a comparison of experimental results obtained under various conditions of MA [9]. Temperature in the vial is also an important parameter influencing MA processes [10 - 12]. It is necessary to know these two parameters to characterise MA process quantitatively.

There are few studies on these parameters experimental determination [13 - 15]. Such procedures, as a rule, are applicable only to some types of mills. For example, the estimation of temperature of MA in the planetary mill can be carried out only indirectly [14]. Such estimations have low precision. Therefore computation of these parameters has wide acceptance [16 - 22].

The aim of the present study is to determine the energy dissipation and average temperature in the vial of planetary ball mill and analyse their dependences on various parameters of MA process, such as the filled fraction of a vial, size of balls, their mass and thermal conductivity.

## PROCEDURE OF SIMULATION

The theoretical grounds of the used model were described previously [21, 22], here only its main concepts are presented.

The ball motion was considered within the limits of planar model, i.e. for the case when vial height equals ball diameter and only one ball layer can be accommodated inside the vial. Such approximation is valid in the case, when all used balls are of the same diameter. The layerwise character of ball motion in planetary mill was recorded photographically [23]. The horizontal grooves on the wall of vial, a distance between which is equal to ball diameter, and which are absent when the balls of different diameter are used [22] may be an additional confirmation of the validity of this approximation. To determine a total energy dissipation in the vial, it is necessary to multiply an energy dissipation in one layer by the number of layers, in which the balls move.

Centre of vial was accepted as the origin of co-ordinates. The trajectories of ball motion in the

field of two centrifugal forces and Coriolis force were computed. The gravity force was neglected due to the fact that the acceleration of milling bodies in the mills of this type is 25 - 60 times greater than free fall acceleration [6]. The velocities of balls after collisions were calculated using the elastic coefficient of centric impact, determined as a portion of kinetic energy, which is conserved under the head-on impact, and also the coefficient of sliding friction, which is equal to a ratio between tangential and normal components of force of response during a short time of collision.

The determination of energy dissipation was carried out by summation of energy losses of each ball per unit time at collisions with vial wall or with other balls. A distinctive feature of calculations given in the present work is the consideration of the ball rotation energy, which, as has appeared, makes a significant contribution to total energy of the system, especially for balls of large diameters. The energy loss is equal to a difference between the kinetic energy of the ball before and after collision, that is $\Delta E = E - E'$.

For the case of ball collision against the vial wall we obtain:

$$\Delta E = \left[\frac{m}{2}(v_n^2 + v_t^2) + \frac{I}{2}\omega^2\right] - \left[\frac{m}{2}((v_n')^2 + (v_t')^2) + \frac{I}{2}(\omega')^2\right],$$

where $m$ is a ball mass, I is the longitudinal momentum of inertia of a ball, $v_n$ and $v_\tau$ are the normal and tangential components of ball velocities, $\omega$ is the angular ball rotation frequency (hereafter the primed and unprimed symbols indicate quantities after and before collision, respectively).

For the case of collision of two balls, a centre of their masses was chosen as the co-ordinate origin. Thus, the energy loss of ball pair as a result of impact is:

$$\Delta E = \left[2\frac{m}{2}(v_n^2 + v_t^2) + \frac{I}{2}\omega_1^2 + \frac{I}{2}\omega_2^2\right] - \left[2\frac{m}{2}((v_n')^2 + (v_t')^2) + \frac{I}{2}(\omega_1')^2 + \frac{I}{2}(\omega_2')^2\right],$$

where $v_n$ and $v_\tau$ are the normal and tangential components of relative velocity of balls, respectively, $\omega_1$ и $\omega_2$ are the angular frequencies of the first and second ball, respectively.

To calculate the temperature in a vial, it was supposed that the heat exchange occurs only through the contact area at collision of balls. Determination of contact area and time was carried out within the framework of the theory of elasticity. An increase of the contact area in the case of ball collision against the vial wall due to a difference between the radii of curvature of a wall and ball was also taken into account. Heat exchange through the gas environment in the vial was neglected due to the fact that heat conductivity of gas is 3 - 4 order less than that for metal materials of balls and vial.

To simulate the heating of balls, it was supposed, that portions of heat, which are liberated at collisions, are spread over bulk of ball immediately, and lead to its uniform heating or cooling.

To determine an average temperature in the vial, the superposition of the solutions of uniform and nonuniform equations of thermal conductivity was employed.

On the basis of this model, a computer program for calculations was formulated. Calculations of energy parameters were performed with a time step of $10^{-4}$ s. The starting velocities of balls were taken as zero. On the initial stage of computation, the high values of energy dissipation, which are caused by irregular interactions of balls, were observed; but a short time later, when the motions of balls became ordered, the energy dissipation decreased and, than, became constant. Time, after which the steady-state conditions were reached, usually lies in the range from 0.3 to 1.5 s depending on the number of balls. The calculated values of energy dissipation and temperature are accepted, if successively computed values have a relative difference of no more than 0,1 %.

Table 1 gives the initial data for computer calculations. All tabulated parameters correspond to a AGO-2U planetary ball mill. Some peculiarities of AGO mill series were described in [24].

**Table 1.** Starting parameters for calculations.

| Parameter | Symbol | Value |
|---|---|---|
| Radius of the planet carrier | R | 50mm |
| Interior radius of vial | $R_{vi}$ | 31mm |
| Exterior radius of vial | $R_{ve}$ | 37mm |
| Rotation speed of the vial | | 37 $s^{-1}$ |
| Rotation speed of the planet carrier | $\nu_p$ | 20 $s^{-1}$ |
| Temperature of cooling liquid | $T_{water}$ | 6 $^0$C |
| Friction coefficient | f | 0.9 |
| Elastic coefficient of centric impact | $\eta$ | 0.25 |

## RESULTS AND DISCUSSION

### 1. Character of ball motion in a vial

As it is known (see, for example, [20]), the character of ball motion depends on the vial occupancy by balls, which is designed by the filled fraction $\xi$. In the two-dimensional model $\xi$ was determined as a ratio of the area, which is occupied by balls, to the total area of vial (in percent). In [20], a relative filled fraction $n_V$, which was determined as a ratio between the number of balls in vial and the greatest possible number of balls, which can be loaded into vial, was used. This coefficient relates with that used in the present study approximately as $n_V = 1{,}27\xi$.

In contrast to the results of [16 - 18], in the case of the presence of a single ball in the vial, its detachment from vial wall was not observed. This divergence is due to the fact that in calculations of [16 - 18], Coriolis force, which affects the tangential acceleration of the ball, was not taken into account.

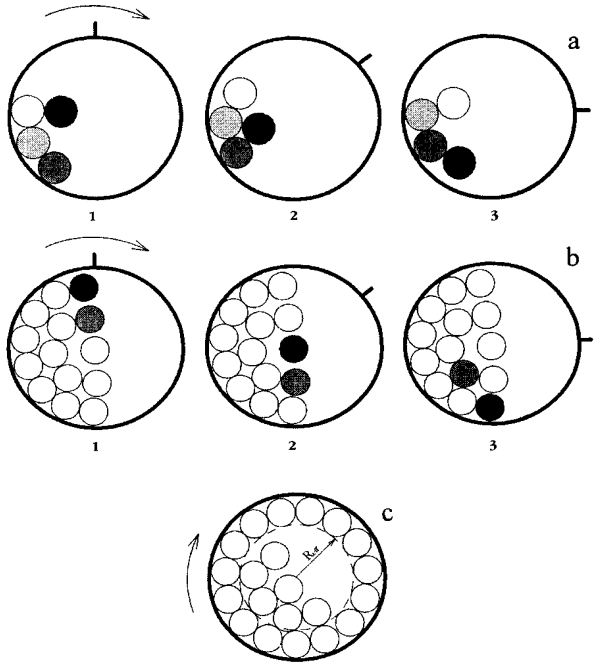


Fig. 1. Schematic representation of ball motion at (a) small (10 - 20 %), (b) medium (40 - 50 %) and (c) high (more than 55 %) values of filled fraction $\xi$.

At small (5 - 10 %) values of filled fraction $\xi$, the «condensation» of balls on a the vial wall in the direction of pseudo-gravity vector, was observed. Figure 1a schematically shows their motion. When the most part of balls is rolled on a vial wall, the balls, which are located on the edge of aggregation, are thrown to the opposite edge. At an increase in $\xi$ to 40-50 %, balls also move as aggregation and performs a cascade transport from one to another edge of an aggregation (Fig. 1b).

When $\xi$ achieves approximately 55 % the smearing-out of aggregation over vial wall begins, what implies the formation of immovable close-packed monolayer of ball coating the wall. Balls in this layer have practically fixed position with respect to the vial. Other part of balls makes a motion in space, which is limited by this layer (Fig. 1c). At such character of motion, only balls which are located beyond monolayer layer, i.e. within effective radius $R_{eff} = R_{vi} - D_b$, participate in the MA process. Hereafter we shall call such behaviour as «spread» effect.

### 2. Dependence of energy parameters of MA process on the filled fraction

Depending on vial occupancy $\xi$, processing materials can be subjected to different types of action with prevailing tangential (at low $\xi$) or normal (at high $\xi$) deformation. In this case, an examination of dependence of energy dissipation E on the filled fraction is of great interest. A variation of $\xi$ was carried out by increasing a number of balls at their constant size.

Figure 2a (curve 1) shows a plot of E vs. $\xi$. It represents a curve with a maximum at a filled fraction of 45-48 %. At $\xi \approx 52\%$, an abrupt decrease in the E was observed. This decrease corresponds to the formation of the first closed shell (Fig. 1c). Dependence of E on $\xi$ by the analytical equation, which was proposed in [16], is presented in Fig 2a, curve 4. These calculated results agree satisfactorily with our data. However, the «spread» effect was not considered in [16]; that is why the curve is continuous.

It is possible, based on known character of the ball motion, to assume a difference between the contributions to the energy dissipation, which are made of frontal collisions (normal component of energy dissipation $E_n$) and glancing collisions (tangential component of energy dissipation $E_\tau$). The obtained dependences (Fig. 2a, curves 2 and 3) testify that at small filled fractions, the dissipation of energy occurs predominantly at the oblique impacts, and at large filled fractions, it occurs primarily at direct impacts. The rise of the «spread» effect at $\xi \approx 52\%$ results in sharp decreases in both $E_n$ and $E_\tau$. A comparison of the contributions of the «ball - ball» and «ball - wall» interactions to the energy dissipation has shown the predominance of the first above the second at all $\xi$.

In general, the obtained data correlate well with the calculated results [20]. The differences may be caused by the fact that summation of energy dissipation in [20] was performed after one revolution of a vial. The model used in the present study gives a more precise result, because it allows to calculate the energy after the steady state conditions are reached.

From these results we can conclude that it is possible to change a character of influence on the processed material considerably by changing $\xi$. At small $\xi$ material will undergo abrading loadings, while at higher $\xi$ the normal deformation prevails.

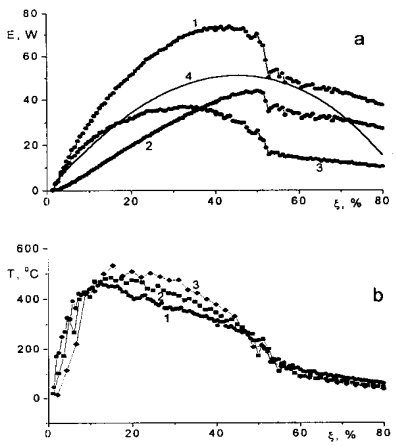


Fig. 2. a - A plot of E vs. $\xi$ varied by raising of ball's number from 1 to 121 ($D_b$ = 4,8 mm): (1) - total value of E; (2) - $E_n$; (3) - $E_\tau$, (4) - E calculated by formula [16].

b - A plot of T vs $\xi$ varied by raising ball's number from 1 to 121 ($D_b$: (1) 4.8, (2) 6.6, and (3) 8.8 mm.

The dependence of temperature on $\xi$ for balls of constant radius (Fig. 2b) is a curve with a maximum at $\xi$ = 15 %. Temperature in a vial depends only slightly on the ball diameter, and it increases with increasing ball diameter.

Comparing the curves on Fig. 2a and 2b, it is seen, that the maxima of E and T do not coincide. The maximum of temperature is located at $\xi$ = 15 %, i.e. in the region where rather high values of energy dissipations are in optimal combination with rather low heat removal.

Thus, to reach the most nonequilibrium state of processed material in the minimum time, it is preferable to treat it at $\xi \sim 45\%$. This mode provides the maximum energy dissipation and rather low temperatures, i.e. can prevent thermal decomposition of the obtained nonequilibrium structure.

**3. Dependence of energy parameters of MA process on the ball size**

The results of calculations allow to analyse an effect of the size of milling bodies on energy dissipation. Figure 3a shows the dependence of energy dissipation on the ball diameter $D_b$. It has a linear character at small $\xi$, when the effect of «spread» is not observed. An increase in E with increasing $D_b$ is caused by the rise of ball mass and hence its kinetic energy (both translational and rotational) because the model under consideration is pseudoplanar: ball is thought of as three-dimensional body. For comparison, Fig. 3a gives the results calculated by the analytical equation [16]. The satisfactory agreement is observed at small and medium values of $\xi$.

At large filled fractions, when the effect of «spread» takes place, the character of dependence of E on $D_b$ changes (Fig. 3a, curve 3). Initially the plot is also linear; however a slope of the curve is much less, than at small and medium $\xi$, because a free path of balls is small at large $\xi$. At high $D_b$, the minimum of energy dissipation was observed. This minimum corresponds to the formation of closed layer of practically fixed balls on the vial wall. A single ball moves within the limits, restricted by $R_{eff}$, as it is shown in a Fig. 1c. The subsequent increase in E is caused by the rise of a free path of balls due to a decrease in their amount ($\xi$ = const), but further increase of $D_b$ leads to a decrease in free path of

balls, i.e. to a decrease in E.

Figure 3b shows a dependence of T on $D_b$. At small $\xi$, it represents a decreasing incremental linear plot for rather large number of balls.

Comparing these values with the experimental data on the dependence of temperature in vial on ball diameter [14], where the value of $\xi$ was about 10-15 %, we may see their good agreement for large sizes of balls. For instance, for $D_b$ = 3 mm, our calculations give 400 $^0$C, and data of [14] - 160 $^0$C, for $D_b$ = 5 mm - 455 and 480 $^0$C, respectively, and for $D_b$ = 9 mm - 520 and 610 $^0$C, respectively.

At large $\xi$, temperature in the vial decreases with an increase in $D_b$ due to a decrease of number of moving balls. Local maxima and minima of temperature correspond to those of energy dissipation.

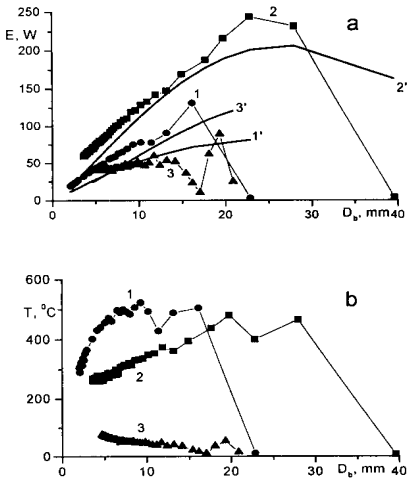


Fig. 3. a - Dependence of E on $D_b$ at $\xi$ (%): (1) 15, (2) 45, and (3) 75. (1', 2', 3') - value of E, calculated by equation [16].

b - Dependence of T on $D_b$ at $\xi$ (%): (1) 15, (2) 45, and (3) 75.

## 4. Dependence of energy parameters of MA process on the material of balls and vial

The ball weight determines its kinetic energy, and, correspondingly, will essentially affect the energy parameters of MA. It is possible to change the ball mass at a constant diameter using the balls of materials with various density.

Figure 4a gives the dependences of E on $\xi$ for various materials of balls and vial. For materials with similar densities, such as Fe, Cr, and alloyed steels, the energy dissipation differs moderately. For a material of balls with density almost twice greater (tungsten carbide WC), the energy dissipation is approximately twice higher and reaches 230 W at $\xi$ = 45%.

An effect of the ball and vial material on temperature is more pronounced than its effect on the energy dissipation. This is due to the differences in the thermal conductivity of chromium, iron and steels that causes the differences in the velocities of ball cooling.

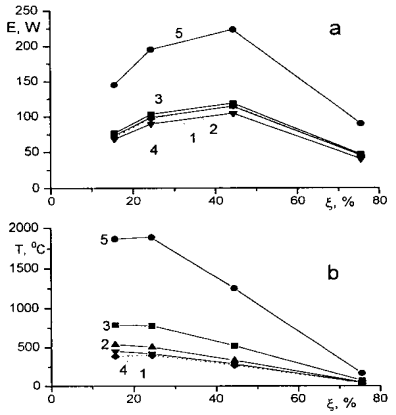


Fig. 4. Dependence of (a) E and (b) T on $\xi$ for various ball's materials ($D_b$ = 8.8 mm): (1) - Fe; (2) - ShKh-15; (3) - 12Kh18N10T; (4) - Cr; (5) - WC.

The dependences of T on $\xi$ for various materials of balls are given in a Fig. 4b. The minimum temperature is observed for iron balls and vial due to a high heat conductivity of iron and relatively large contact area. The contact area and collision duration increase with a decrease of sound velocity (square root of Young's modulus related to material density) in material. An increase of contact area and collision duration lead to an increase of intensity of heat exchange between balls and, thus, reduces their temperature facilitating heat removal to a wall made of the same material. The results obtained for chromium are similar to those for iron; the heat conductivity of chromium is higher, but the contact area and impact time are smaller than that of iron. For balls and vial made of ShKh-15 steel (ball-bearing steel with 1.5 % Cr), the temperature is slightly higher than that for iron and chromium; for this material, the contact area is larger, but heat conductivity is significantly lower than that for iron. In the case of 12Kh18N10T steel (stainless steel containing 18 % Cr, 10 % Ni, ~1 % Ti),

the temperature is considerably higher than for Fe, Cr and ShKh-15 due a low heat conductivity of stainless steel.

Very high temperatures for balls and vial of tungsten carbide are associated with a high energy dissipation of the device made of WC, low heat conductivity of tungsten carbide, and also small radius of contact area during collisions.

Using various materials of balls and vial, it is possible to influence phase composition of the processed materials. This, in particular, can explain the experimental data of [8]. Using the balls and vial of stainless steel in MA of $Mo_{33}Si_{66}$ composition, the authors of [8] observed the formation of β-$MoSi_2$ phase, which is metastable at ambient temperature, and using balls and vial of tungsten carbide, the formation of α-$MoSi_2$ stable phase was observed. This may be a consequence of a higher temperature of processing with tungsten carbide as the material of balls and vial.

## CONCLUSIONS

The performed analysis of milling media behaviour and energy parameters of MA in relation to various processing factors allows to conclude that the character of ball motion in a vial of a planetary ball mill depends strongly on the filled fraction. When it reaches 55 %, a transition take place from a motion of balls in aggregation to the effect of their «spread» on the vial wall. This effect is accompanied by an abrupt decay of energy dissipation and temperature. An increase of the ball's size at a constant filled fraction in most cases results in an increase of energy dissipation and temperature. By varying the filling factor, it is possible to vary the character of action on the material from abrasion to shock strain. The material of balls and vial considerably affects the temperature and energy dissipation.

The obtained results allow to choose the optimal modes of MA process with regard to the specificity of particular problems.

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