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Influence of Thickness of Self-Lined Layer on the Parameters and Kinetics of Mechanical Activation (on Example of Quartz Processing)

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Abstract

The influence of thickness of self-lined layer of processed substances on the parameters of mechanical activation is considered. Theoretically, using quartz as an example, dependencies of impulses of pressure and temperature along the layer thickness are calculated. It is shown that this parameter affects significantly the kinetics of mechanochemical processes.

Key words: mechanical activation, theory, thickness of self-lined layer, modeling

INTRODUCTION

It is known [1, 2] that processes in mechanochemical reactors (MR) in a number of cases do not go to completion. For example, in the process of grinding the establishment of the dynamic equilibrium by sizes of the mechanically activated (MA) particles takes place [3–5], which is a part of a rather well studied concept of "mechanochemical equilibrium" [1, 2, 6, 7]. The existence of the dynamic equilibrium between the processes of fracture and aggregation of particles serves as the basis for the phenomenon of self-lining of the milling tools surface in MR (Fig. 1, *a*) with the thickness (δ) of the self-lined layer [8–10]. In principle, it is similar to the phenomena of compaction and sintering of powders [11], a difference consists only in mechanochemical realisation of these processes in MR. Thus for MA particles of quartz in a planetary ball mill δ may be expressed as follows [12, 13]:

$$\delta = m_1/\rho_1(1-p)(\Pi_v + \Pi_b) \approx 4m_1/\pi\rho_1(\Pi_v + 4\pi R^2 N) \quad (1)$$

Here $\rho_1 = 2590\ \mathrm{kg/m^3}$ is density of quartz; $p \approx 1 - \pi/4$ is porosity of layer; Π_v and Π_b are areas of walls of the mill vial and total surface

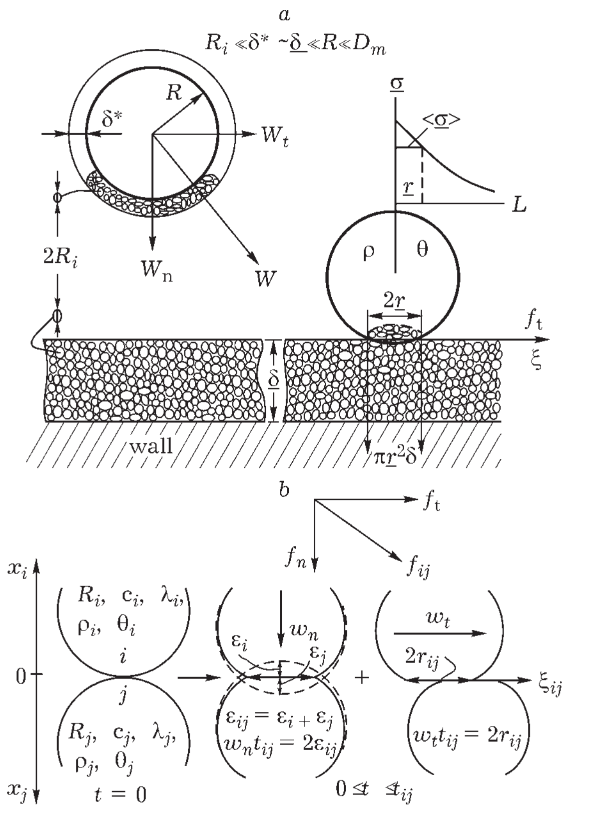

Fig. 1. Scheme of impact-friction interactions of milling tools and MA of particles of quartz: *a* – milling tools; *b* – any contacting particles *i* and *j* from the selected volume $\pi r^2\delta$.

of balls; R and N are radius and number of balls, respectively.

On the other hand, in the studies of MA processes in MR there is the following relationship between mass (m_b) of mobile milling tools (ball load for all types of ball mills) and mass (m_1) of MA substance [1, 2, 14, 15]: $m_b/m_1 >> 1$. As a rule, this value (m_b/m_1) is about 50 (there is about 2 g of the processed material per 100 g of the ball load). Such a choice of the value of m_b/m_1 is related to that at its considerable decreasing, the processes of MA in MR do not go to completion or they require unjustified long time of MA, to complete the process of mass transfer in MR [16]. At increasing m_b/m_1 the consumption of mechanical energy becomes unjustified per unit of mass m_1 of MA substance. As $m_b = 4\pi R^3\rho N/3$, where ρ is ball density, then (1) is written as:

$$\delta = m_1/\rho_1(1-p)[\Pi_v + (3m_b/\rho R)]$$
$$\approx 4m_1/m_b\pi\rho_1[(\Pi_v/m_b) + (3/\rho R)] \sim m_1/m_b \quad (1a)$$

Expression (1a) shows inversely proportional dependence of ratio δ and m_b/m_1.

The action of the ball load on quartz particles is carried out through the layer δ with relative velocity (W) of collisions between milling tools (see Fig. 1, *a*). The value W of collisions between milling tools is given by the equation:

$$|W| = 2\pi\omega D_1[(\kappa+1)^2 + \Gamma^2 - 2\Gamma(\kappa-1)\cos\varphi + (\Gamma+1)^2]^{0.5} \quad (2)$$

$$W_n = |W|\sin\varphi \text{ and } W_t = |W|\cos\varphi \quad (3)$$

where $\cos\varphi = -(1+\kappa)/\Gamma$, determines the angle of ball rebound from walls. The geometric factor $\Gamma = D/D_1$, where D and D_1 are the radii of the carrier and vial, respectively; the kinematic factor $\kappa = \boldsymbol{\omega}_1/\boldsymbol{\omega}$, where ω_1 and ω are the number of revolutions of the vial and the opposite number of carrier revolutions, respectively. An analysis of the interaction of milling tools must be performed taking into account both the normal component W_n and the tangential component W_t of the W. The value of W_n determines the conditions of the interaction of particles in the layer. The value of W_t determines the conditions of mechano-chemical processes on the frictional contact between milling tools and treated particles.

In [12, 13] the process of MA of quartz in the steel ball three-cylinder planetary mill produced by "Mekhanobr" Co. (St. Petersburg) was studied, the characteristics of the mill were: $\Gamma = D/D_1 = 2.3$, $D = 0.115$ m and $D_1 = 0.05$ m; $\kappa = \boldsymbol{\omega}_1/\boldsymbol{\omega} = -1.7$, $\omega_1 = 20$ s^{-1} and $\omega = 11.7$ s^{-1}; $W \approx 17$ m/s, $W_n \approx 5$ m/s, $W_t \approx 16$ m/s; the cylinder volume $V = 0.00045$ m^3; and the working part of the vial surface $\Pi_d = \pi D_1(2h + D_1) \approx 0.025$ m^2, where $h = 0.055$ m is the vial height. The ball radius was $R = 0.005$ m, ball density $\rho = 7800$ kg/m^3, number of balls $N = 120$, their total surface $\Pi_b = 4\pi R^2 N \approx 0.037$ m^2.

The ratio of m_b to the mass of MA quartz m_1 was equal to 4 at $m_b + m_1 = 0.6$ kg. Calculation on eq. (1a) gives $\delta \cdot 10^{-3}$ m, which is more than an order of magnitude greater than for traditional values m_b/m_1 or $\delta = 10^{-4}$–10^{-5} m, accepted in the calculations of kinetics of mechanochemical processes [10]. Theoretical description of MA of quartz is presented in [12, 13]. Calculations were conducted for "equilibrium" radius of quartz particles $R_1 = 3 \cdot 10^{-7}$ m [3] without considering the effect of the thickness of self-lined layer δ of the processed substances on the parameters and kinetics of MA. Therefore, for the traditionally accepted MA time (up to 90 min), the reaction of iron oxidation of abrasive wear of milling tools with subsequent formation of iron silicates on the surface of quartz particles proceeds incompletely – no more than by ~10 % [12, 13].

MODELING PROCEDURE

Thus, it is possible to state the possibility of substantial influence of value δ on the parameters and kinetics of processes of MA of quartz at m_1 relatively close to m_b. Below we make the first attempt to introduce the value δ for the theoretical estimation of the parameters of MA substances for the example of the quartz treatment according to above-presented method.

It is known [17] from powder pressing theory that the key parameter – mechanical stress σ on the impact-friction contacts of milling tools and MA particles – must depend on the thickness of the pressed powder-like material:

$$\sigma(h) = \sigma_0 \exp(-2\eta\xi h/r) \quad (4)$$

where $0 \le h \le \delta$ is variable h on the thickness of pressing δ; σ_0 is pressure of pressing; r is pressing radius; η is coefficient of lateral pressure; ξ is coefficient of external friction.

Impulse of the pressure of pressing σ_0 on the surface ($h = 0$) of ball impact with the flat layer of MA particles of quartz on the vial wall is described by expression [10]:

$$\sigma_0 = (8/3\pi)(10\pi)^{0.2}[\rho(\theta + \theta_1)^{-4} W_n^2]^{0.2} \quad (5)$$

Here $\theta = 4(1 - \nu^2)/E = 1.65 \cdot 10^{-11}$ m^2/N and $\theta_1 = 4(1 - \nu_1^2)/E_1 = 3.95 \cdot 10^{-11}$ m^2/N are compliance coefficients; $\nu = 0.85$ and $\nu_1 = 0.302$ are the Poisson's coefficients; $E = 2.23 \cdot 10^{11}$ N/m^2 and $E_1 = 0.983 \cdot 10^{11}$ N/m^2 are the values of Young's modulus for steel and quartz, respectively.

The force (f) of interaction of milling tools and radius (r) of the contact surface are determined from expressions:

$$f = 2/3(10\pi)^{0.6}R^2\rho^{0.6}(\theta + \theta_1)^{-0.4} W_n^{1.2} \quad (6)$$

$$r = 1/2[(3/2)f(\theta + \theta_1)R]^{1/3} \quad (7)$$

The results of the calculations according to (4)–(7) at $\eta = 1$ (coefficient of lateral pressure for polycrystalline material [17] is used in [10] and it characterizes flat layer [8–10]); $\xi = 0.3$ (accepted for dynamic friction coefficient of iron on quartz [18]) are illustrated in Fig. 2.

Temperature impulse $\Delta T(h, t)$ on the impact-friction contact of a ball with flat self-lined layer of quartz particles (see Fig. 1, *a*) is described by expression [10]:

$$\Delta T(h, t) = \xi\sigma(h)W_t(cc_1\lambda\lambda_1\rho\rho_1)^{-0.25}\{t^{0.5} iErfc[h/2(a_1t)^{0.5}] - (t - \tau)^{0.5} iErfc[h/2a_1^{0.5}(t - \tau)^{0.5}]\} \quad (8)$$

Here $\lambda = 75.3$ W/(m · K) at 773 K and $\lambda_1 = 7.7$ W/(m · K) at 673 K; $c = 667$ J/(kg · K) at 773 K, $c_1 = 1250$ J/(kg · K); $C_p = 76$ J/(mol · K) at 844 K, *i. e.* at the point close to $\alpha \leftrightarrow \beta$ transformation in quartz; $a = \lambda/(\rho c) = 1.45 \cdot 10^{-5}$ m^2/s and $a_1 = \lambda_1/(\rho_1 c_1) = 2.38 \cdot 10^{-6}$ m^2/s are thermal conductivities, specific heat capacities and thermal diffusivities for steel and quartz, respectively; and $\tau = (\pi/4)[10\pi\rho(\theta + \theta_1)]^{0.4}R\, W_n^{-0.2}$ is the time of impact-friction interaction. In particular, the section $\Delta T(h, t = \tau)$ is the change of maximal value of temperature on the thickness of flat layer of quartz particles is presented in Fig. 3. It is evident that a sharp decrease of temperature takes place along the thickness of layer (only near-surface particles are warmed up).

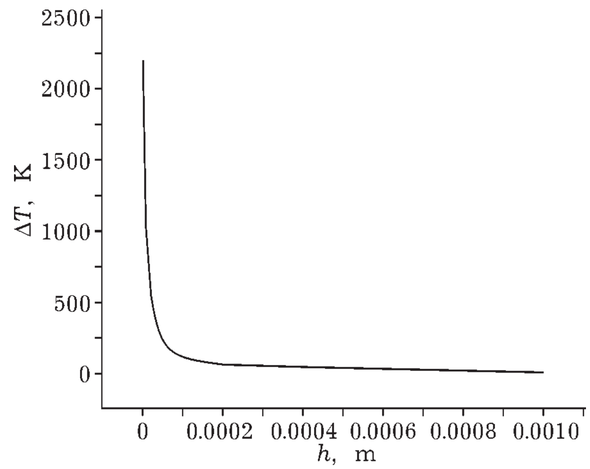

Fig. 3. Temperature impact distribution (ΔT) on a thickness (h) layer of quartz particles.

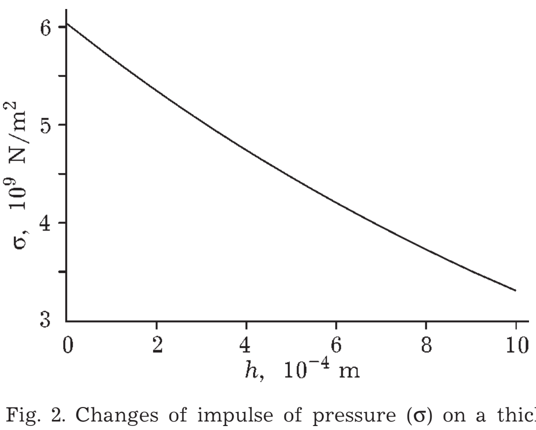

Fig. 2. Changes of impulse of pressure (σ) on a thickness of flat layer (h) of quartz particles.

Local heating $\Delta T(x, h, t)$ of quartz particles in the volume of self-lined layer takes place on impact-friction contacts as a result of impulse of pressure $\sigma(h)$ while it passes through the layer. In the calculations, we do not take into account deviation x from the contact plane deep into the quartz particles (see Fig. 1, *b*), *i.e.* it was accepted that $x = 0$. To derive the formula for $\Delta T(h, t)$, it is necessary to revise the formulae developed for parameters of MA of particles in the volume of self-lined layer [10, 12, 13] and bind them with $\sigma(h)$. Now the force f_1 of interaction of quartz particles will be determined by expression:

$$f_1(h) = (f/s) = s_1(h)\sigma(h)$$

where $s_1 = \pi r_1^2$ is the impact area of the contact of particles, and $s = \pi r^2$ (see eq. (7)). Then $s_1(h)$ is derived from expression

$$s_1(h) = (\pi/4)[(3/2)\sigma(h)s_1(h)\theta_1R_1]^{2/3}$$

as follows:

$$s_1(h) = (\pi/4)\,[(3\pi/8)\sigma(h)\theta_1R_1]^2 = \pi\langle r_1(h)\rangle^2 \quad (9)$$

Knowing $s_1(h)$ we find $f_1(h) = [\sigma(h)\pi/4]^3[(3/2)\theta_1R_1]^2$ and other parameters of MA of particles:

(i) total deformation (approach) of contacting particles of quartz (see Fig. 1, b):

$$2\varepsilon_1(h) = 2R_1[\sigma(h)\theta_1 3\pi/8]^2 \qquad (10)$$

(ii) time τ_1 of particles interaction is determined from expression $\tau_1(h) = 2\varepsilon_1(h)/w_n = 2r_1(h)/w_t$, where normal velocity w_n we will find from $2\varepsilon_1(h)/w_n = (\pi/4)(10\pi)^{0.4}[w_n^{-1}\, 2(\rho_1 R_1 \theta_1)^2]^{0.2}$ and w_n is determined as:

$$w_n = (2^{0.5} 10\pi\rho_1 R_1^{2.5}\theta_1)^{-0.5}[8\varepsilon_1(h)/\pi]^{1.25}$$
$$= (9\pi)^{1.25}\theta_1^2 <\sigma(h)>^{2.5}/16(10\pi\rho_1)^{0.5} \qquad (11)$$

(iii) using (9)–(11), we find $\tau_1(h)$ and tangential component $w_t(h)$ of particles (Figs. 4, 5):

$$\tau_1(h) = 2\varepsilon_1(h)/w_n = [5\pi^{2.5}\rho_1 R_1^2/2^{0.5}3\sigma(h)]^{0.5} \qquad (12)$$

$$w_t(h) = 2r_1(h)/\tau_1(h) = (3/8)[2^{0.5}3<\sigma(h)>^3\theta_1^2/5\pi^{0.5}\rho_1]^{0.5} \qquad (13)$$

Using (12) and (13) we determine the desired impulse of temperature on the surface ($x = 0$) of the particles (see Fig. 1, b):

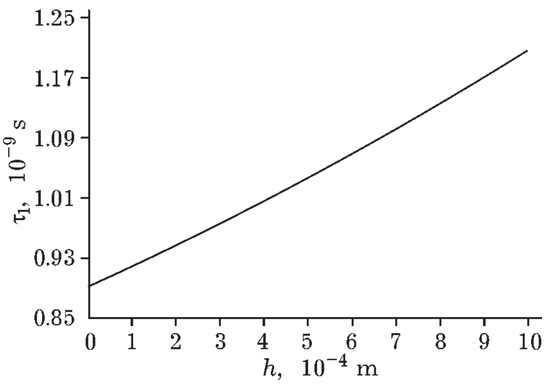

Fig. 4. Time change of interaction (τ_1) of quartz particles on a thickness of flat layer (h).

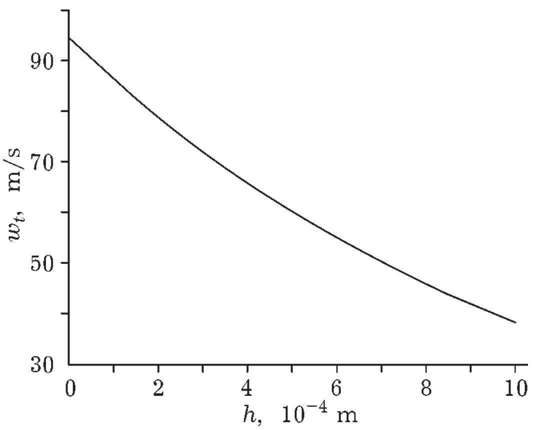

Fig. 5. Changes of tangential velocity (w_t) of interaction of particles on a thickness.

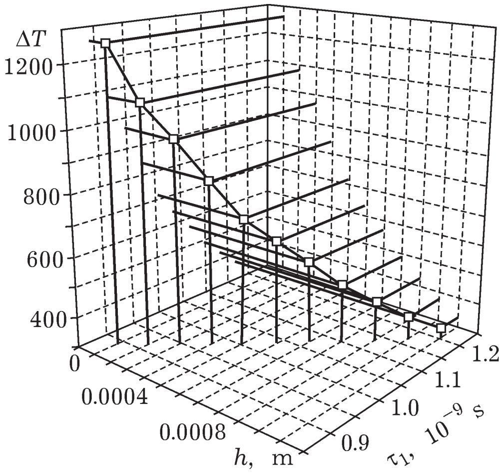

Fig. 6. Changes of impulse of temperature ΔT along the thickness (h) and within time (τ_1).

$$\Delta T(h,\ x = 0,\ t) = iErfc[0]\xi_1\sigma(h)W_t(h)(c_1\lambda_1\rho_1)^{-0.5}$$
$$\times\{t^{0.5} - [t - \tau_1(h)]^{0.5}\} = 0.5642\xi_1(3/8)$$
$$\times[2^{0.5}3<\sigma(h)>^5\theta_1^2/5\pi^{0.5}]^{0.5}(c_1\lambda_1\rho_1^2)^{-0.5}$$
$$\times|t^{0.5} - \{t - [5\pi^{2.5}\rho_1 R_1^2/2^{0.5}3\sigma(h)]^{0.5}\}^{0.5}| \qquad (14)$$

Here $iErfc[0] = 0.5642$; $\xi_1 = 0.65$ is the coefficient of dynamic friction between quartz particles [19, 20]. Calculations of the most meaningful sections of impulse of temperature $\Delta T(h, t)$ on the friction contact of quartz particles are presented in Fig. 6:

– on the lower plane there is the section along h and corresponding values τ_1 (see Fig. 4);

– on a right lateral plane the section $\Delta T[h, \tau_1(h)]$ is given against thickness h of self-lined layer;

– on the left plane the section $\Delta T[h(\tau_1), \tau_1]$ is given against time τ_1 of interaction of quartz particles.

CONCLUSION

The performed calculations point to substantial influence of the thickness of self-lined layer on the parameters of MA of the substances processed in a planetary mill and, as a result, on the kinetics of mechanochemical processes. We should mark that the thickness of self-lined layer of the processed material is totally determined by the mass of charge and by the surface area of milling tools (walls of vial and ball load).

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