Study of the Temperature Variations of AI and Ti in Mechanical Alloying

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This study aims to corroborate experimental studies in mechanical alloying by theoretical studies, particularly the calculation of the contact temperature at the impact point of the balls, basing on the mathematical model of a compact powder between two colliding balls. Indeed, within this study, we show the influence of some geometrical, dynamic, and thermophysical parameters on the variation in the contact temperature of balls and Al and Ti powders inside a vial of planetary ball mill.

Keywords contact temperature, parameters of milling, planetary ball mill

1. Introduction

Mechanical alloying or high-energy milling (Ref 1, 2), is a process which permits, by means of repeated shocks between balls and a tightly enclosed powder, to obtain new nano-metric materials in a meta-stable state. Experimentally, the determination of the ball-powder temperature of contact is very difficult to evaluate. For this reason, we propose in this article a method to determine the contact temperature by mathematical models. It is admitted that in the process of mechanical alloying, adjustment of the following parameters: velocity ratio, vial radius, the distance between center of disk and center of vial, and rotation direction, allows obtaining a greater energy of impact. Throughout our study, it is admitted that the kinematic analysis of the ball is in a Cartesian plan in relation to the rotation of both the vial and the disk (Ref 3, 4).

2. Flight Velocity of the Ball

The ball is assimilated to a projectile with an initial velocity which is its own take-off velocity. Figure 1 shows the position of a ball materialized by M point in a Retsch PM 400 planetary mill. Considering R_b as the ball radius with, $r^* = r - R_b$, the flight velocity of the ball can be written as follows (Ref 5):

$$\|\vec{V}_{a}\| = \sqrt{(R\Omega)^{2} + (r^{*}\omega)^{2} + 2R\Omega\omega r^{*}\cos\left(\arccos\left(-\frac{r^{*}\omega^{2}}{R\Omega^{2}}\right) + 2\theta\right)}$$
(Eq 1)

where *R* is the distance between center of disk and center of vial, *r* the vial radius, α the angle between the distances *R* and *r*, Ω the angular velocity of the disk, ω the angular velocity of the vial, and θ the rotational angle of the disk ranging from 0 to 2π .

3. Thermal Modeling in Mechanical Alloying

In mechanical alloying, fragments of powder particles are caught between the colliding balls and the wall of the vial in a planetary ball mill (Ref 6, 7). The impact time is estimated by the hertzian theory of the elastic impacts (Ref 8). The compact powder might be represented by a disk thickness t_0 and radius r_0 (Ref 9). The latter can be regarded as the radius of the contact surface of the two balls which are in elastic collision. On the one hand, the kinetic energy of the balls is dissipated in elastic strain; on the other hand, the energy of the compact powder is dissipated in plastic deformation.

Total kinetic energy for each ball is

$$E_{\rm c} = \frac{1}{2}mv^2 \tag{Eq 2}$$

with *m* being the mass of the ball in kg, and v the ball velocity at the moment of the impact in m/s.

The analysis, carried out by Maurice and Courtney (Ref 10), shows that only a small fraction ψ of the supplied energy is used in the plastic deformation process.

This energy is represented by the equation below:

$$U_{\rm p} = \psi E_{\rm c} \tag{Eq 3}$$

with ψ being the plastic deformation coefficient of the ball, and E_c the kinetic energy of the ball in J.

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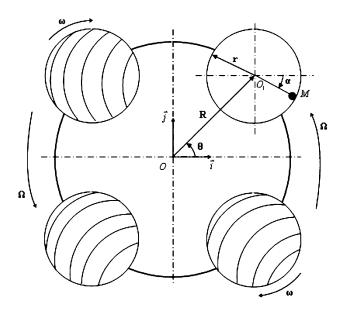


Fig. 1 Geometry of a Retsch PM 400 planetary ball mill

Q, an equivalent heat quantity, appears at each zone of contact. Indeed, one might consider that the ball is a semiinfinite body owing to the fact that the contact surface during the impact is very small as compared with the total surface of the ball (Ref 8). At t = 0, the provided heat flux is

$$q_1 = \frac{(1-\delta)Q}{\pi r_0^2 \Delta \tau} \tag{Eq 4}$$

 $(1 - \delta)$ being the fraction produced within the ball and *Q* the average quantity generated by the total deformation after a $\Delta \tau$ period. The contact temperature is given by (Ref 8)

$$T_{\rm c} = T_0 + \frac{2q_1\sqrt{\alpha_{\rm s}\Delta\tau}}{K_{\rm s}} \bigg\{ \frac{1}{\sqrt{\pi}} - \operatorname{ierfc} \frac{r_0}{2\sqrt{\alpha_{\rm s}\Delta\tau}} \bigg\}$$
(Eq 5)

with T_0 , being the room temperature in K; α_s the thermal diffusivity of the ball in m²/s; K_s the thermal conductivity of the ball in J/s m K; and ierfc the integral of the complementary error function.

 $\Delta \tau$, the impact time, and r_0 , the contact radius, are represented by the Eq 6 and 7:

$$\Delta \tau = 2.787 \nu^{-0.2} \left(\frac{\rho_{\rm s}}{E}\right)^{0.4} R_{\rm b} \tag{Eq 6}$$

$$r_0 = 0.9731 v^{0.4} \left(\frac{\rho_{\rm s}}{E}\right)^{0.2} R_{\rm b} \tag{Eq 7}$$

with *E* being Young' modulus in N/m², and ρ_s the ball density in kg/m³.

Heat flow shape in the compact powder may be modeled by a one-dimensional plate on a surface $x = t_0/2$, with a heat flux q_2 given by the equation below:

$$q_2 = \frac{\delta Q}{\pi r_0^2 \Delta \tau} \tag{Eq 8}$$

with δ being the heat fraction produced inside the powder; *Q* the average quantity generated by the total deformation process in J; r_0 the radius of the compacted powder in m; and $\Delta \tau$ the impact time in s.

For symmetrical reasons of Ref 8, no heat flow crosses through the mid plan. For the same reasons, one will neglect the

Table 1Thermophysical properties of balls and powders(Ref 12, 13)

Materials	Thermal conductivity, W/m K	Specific heat, J/kg K	Density, kg/m ³	Young modulus, N/m ²
Aluminum	238	917	2700	
Titanium	16	528	4500	
Stainless steel (balls)	16	120	7800	1.79×10^{11}

temperature losses from the free ends of the compact powder, which is true because of $2r_0/t_0$ ratio size. Temperature distribution, at the end of the impact (Ref 8), is given by the Eq 9 below. In order to determine δ , the shared heat fraction between the compacted powder and the ball, relations (5) and (9) are equalized.

$$T_{c} = T_{0} + \frac{2q_{2}\Delta\tau}{\rho_{c}C_{p}t_{0}} + \frac{q_{2}t_{0}}{2K_{c}} \Biggl\{ \frac{1}{3} - \frac{2}{\pi^{2}} \sum_{n=1}^{\infty} \frac{(-1)^{n}}{n^{2}} \exp\left(-\frac{4n^{2}\pi^{2}\alpha_{c}\Delta\tau}{t_{0}^{2}}\right) \cos(n\pi) \Biggr\}$$
(Eq 9)

Considering the ball-ball impact T_c , the contact temperature, at the end of the impact, then becomes (Ref 8):

$$T_{\rm c} = \frac{Q}{2\pi r_0^2 \rho_{\rm s} C_{\rm ps} \sqrt{\pi \alpha_{\rm s} \Delta \tau}} \bigg\{ 1 - \exp\left(-\frac{r_0^2}{4\alpha_{\rm s} \Delta \tau}\right) \bigg\}$$
(Eq 10)

with C_{ps} being the specific heat of the ball in J/kg K.

4. Discussion and Results

Several studies show that in mechanical alloying, temperature rise plays a very significant role upon the phase structure induced by milling. Some authors (Ref 11) have determined the temperatures either directly by infrareds measurements or indirectly by knowing those of phase transformations or diffusion coefficients. Our study aims at calculating the contact temperature between ball and powder while varying geometrical, dynamic, and thermophysical parameters (Table 1).

The values of Al and Ti powders and stainless steel balls, were taken from the references (Ref 12) and (Ref 13) in 0 to 100 °C temperature interval, but in our case the specific heat of balls was changed by increasing its value given in Table 1 for optimal milling temperature corresponding to, Young's modulus E and plastic deformation coefficient ψ , respectively for proper steel which constitute the balls. The density and thermal conductivity of the balls remain unchanged.

4.1 Milling Conditions

The used planetary ball mill is a "PM 400" type. Its main characteristics are: vial diameter Dj = 85 mm; distance between center of disk and center of vial R = 150 mm; vial volume $V_j = 500$ mL; plastic deformation coefficient of the ball, $\psi = 0.043$; and rotational speed of the disk, $\Omega = 220$ tr/mn.

The thermophysical properties of balls and Al and Ti powders are discussed in the following.

4.2 Experimental

4.2.1 Ball-Powder Temperature of Contact Varying According to the Impact Velocity. Figure 2 represents the variation in the ball-powder temperature of contact according to the impact velocities of the balls with two materials namely: Aluminum and titanium. A temperature rise is observed, ranging from the minimum of 222.35 °C (Aluminum) to the maximum of 350 °C (Titanium).

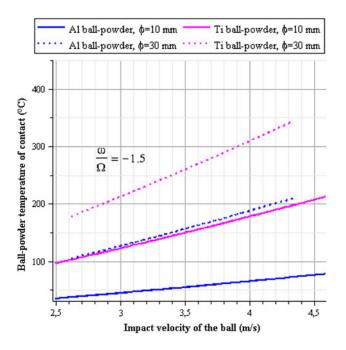


Fig. 2 Ball-powder temperature of contact varying according to the impact velocity of the ball for one revolution of the disk of the planetary mill with ball diameters ($\emptyset = 10$ and 30 mm)

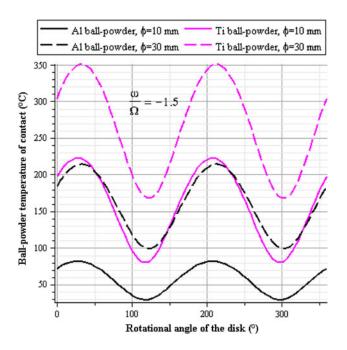


Fig. 3 Al and Ti ball-powder temperatures of contact varying according to the rotational angle of the disk of the planetary mill with ball diameters ($\emptyset = 10$ and 30 mm)

Indeed, elementary or pre-alloyed powders milling results in energy transfer from the milling tools (balls and walls of the vial) to the powders. One of the characteristics of mechanical alloying is the presence, within the impacted powders, of important densities of defects and inner stresses (Ref 14). The latter permit a rise in the free energy of the particles and a temperature rise mainly due to an adiabatic transformation of the deformation work, in addition to the transformation of compression stress or shear stress in calorific energy (dissipation of the energy by Joule effect).

4.2.2 Variations in the Ball-Powder Temperature of Contact According to the Rotational Angle. Figure 3 represents the variation in the ball-powder temperature of contact, according to the rotational angle of the disk. A "tick slip" alternating behavior and self-reproducing temperature variations are observed during the whole experiments over a 180° period. Temperature increases to reach maximum values with optimal rotational angles, and then decreases at close rotational angles.

This might be explained by the variations in the kinetic energy of shock depending on the impact velocity which depends itself on the rotational angle of the disk. At maximum temperatures, the balls, while rolling across the inner surface of the vial, are pressed against the wall of the vial by a significant centrifugal force. The balls mill the powder producing a refinement and considerable defects of the structure. On the other hand, lower temperatures correspond to a less intense centrifugal force. As a result, the balls knock at the bottom of the vial to get an effective milling. This phenomenon enables us to explain and confirm J. Benjamin's theory (Ref 7), suggested in the 1970s, in which he stated that mechanical alloying is ruled by two stapes: the first one corresponds to intensive milling, and the second to the refinement of the obtained structure.

4.2.3 Temperature Variation According to the Distance from Mill Axis to Vial Axis (*R***).** Figures 4 and 5 represent the variation in the contact temperatures between balls and Ti

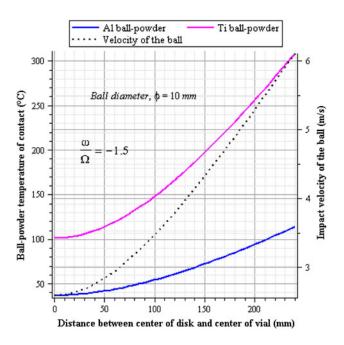


Fig. 4 Contact temperatures between balls and Ti and Al powders and impact velocities of the balls according to *R* with a rotational velocity ratio: $\omega/\Omega = -1.5$ and a ball diameter, $\emptyset = 10$ mm

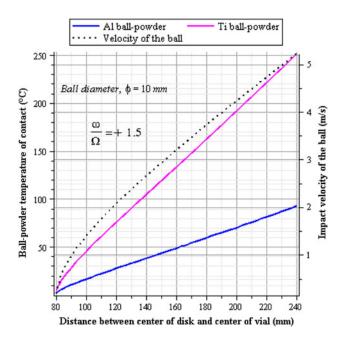


Fig. 5 Contact temperatures between balls and Ti and Al powders and impact velocities of the balls varying according to *R* with a rotational velocity ratio: $\omega/\Omega = +1.5$ and a ball diameter, $\emptyset = 10$ mm

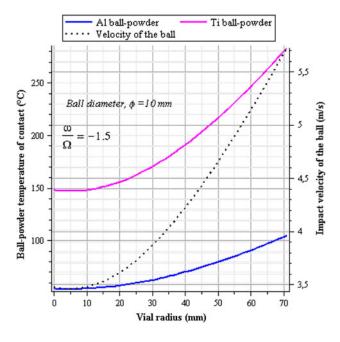


Fig. 6 Contact temperatures between balls and Ti and Al powders and impact velocities of the balls varying according to the vial radius with a rotational velocity ratio: $\omega/\Omega = -1.5$ and a ball diameter, $\emptyset = 10 \text{ mm}$

and Al powders as well as the impact velocity of the balls according to the variation of *R* (distance between center of disk and center of vial). The study was carried out by taking into account the rotational velocity ratios: $\omega/\Omega = +1.5$, $\omega/\Omega = -1.5$, and a vial diameter: 85 mm.

One can notice that the contact temperatures and the impact velocities are proportional to R (the distance from mill axis to vial axis). The latter can be regarded as a leverage needed

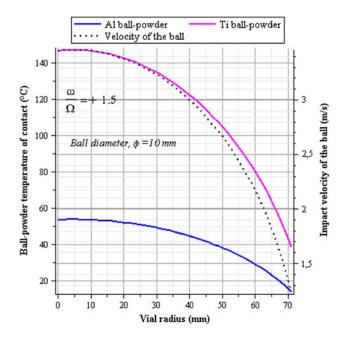


Fig. 7 Contact temperatures between balls and Ti and Al powders and impact velocities of the balls varying according to the vial radius with a rotational velocity ratio: $\omega/\Omega = +1.5$ and a ball diameter, $\emptyset = 10$ mm

to create a moment capable to encourage a more significant disk rotation. The contact temperature between ball-ball and ball-powder increases with the kinetic energy of impact. The latter is due to an adiabatic conversion of the deformation work and consequently, allows an increase in the shock power.

4.2.4 Variation of the Vial Radius. To complete our study, we changed the vial radius. Figures 6 and 7 show the variations in the contact temperatures of the balls with Al and Ti powders of aluminum and titanium, respectively, as well as the impact velocities of the balls, according to the variation of the vial radius with rotational velocity ratios ± 1.5 .

From the above figures, one can notice that the variation in the contact temperatures and the impact velocities are proportional to the vial radius as the velocity ratio is negative $(\omega/\Omega = -1.5)$. On the contrary, they are inversely proportional as the same ratio becomes positive.

This phenomenon may be explained by the definition of the impact velocity of the balls. Indeed, the velocity depends on the vial diameter $(2R_j)$ and the relative angular velocity $(\Omega - \omega)$. It is given by the following relation:

$$V_{\rm r} = \frac{D_{\rm j} - D_{\rm b}}{2} (\Omega - \omega) \tag{Eq 11}$$

with D_j being the vial diameter; D_b the ball diameter; and (Ω ω) the angular velocity of the vial.

It is interesting to note that when the rotational ratio is negative, ($\omega/\Omega = -1.5$), the relative velocity of the ball varies according to (2.5 Ω). On the other hand, when the rotational ratio is positive, the same velocity varies according to (0.5 Ω).

The above results show that it is not only choosing a negative velocity ratio does not make milling more effective. Vials with bigger diameters are needed. Indeed, under experimental conditions, it has been shown that the bigger the vial diameter is, the higher the balls will bounce. Consequently, the more the energy will be dissipated.

5. Conclusion

This study shows that an obtaining nano-metric material by mechanical alloying process is not only the fruit of an intensive milling but also the result of an adequate temperature rise.

Indeed, the contact temperature of the powders depends on the variation of the thermo physical, geometrical, and dynamic parameters of milling.

First obtained results show that

- The contact temperatures between ball and powder increase according to the impact velocities.
- There is an alternating temperature behavior while the disk is rotating.
- *R* (the distance from mill axis to vial axis) is a quality criterion to select a planetary ball mill.
- The bigger the vial radius is, the more the energy is dissipated.

In future studies, we envisage to do experiment studies to validate our above obtained numerical results.

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