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TEMPERATURE RISE DURING MECHANICAL ALLOYING

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Introduction

Mechanical alloying has been well developed to the level of industrial application for manufacturing a wide range of materials, including ODS alloys (1-3), intermetallics (4,5), solid solution alloys (6,7) and amorphous materials (8,9). In spite of this progress, research efforts to understand the basic operating mechanisms during the process of mechanical alloying have been very limited. Understanding the heat dissipation during alloying is one of them. It is very likely that the temperature rise of the powder compact caused by the impacting grinding media could play a central role in most of these operating mechanisms, particularly for diffusion to take place during alloying. However, the efforts (8, 10-11) to describe the heating effects during MA are often based on assumptions related to bulk impacted material and therefore, may not represent the true maximum temperature at the areas close to impact. This note is an attempt to provide calculations for the temperature rise from different points of view, which seem to indicate that indeed in the mechanical alloying process, a significant increase in localized temperature is a likely event.

Model and Analysis

During the beginning of mechanical alloying processing sequence, ball to ball impact traps many powder particles between them. Atomically clean interfaces (1) are thus brought into intimate contact, forming cold welds between the powder particles and building up layered composites of flattened particles in the form of a compact. The size of such a compact, containing many particles, is an evolving parameter, and depends on the balance between cold welding and subsequent fracturing events. Eventually, these compacts reach a steady state size.

a) Increase in contact temperature during impact

First of all, for modelling a collision of such a powder compact between two spherical balls, we will make the following two fundamental assumptions; a) the time of impact $\Delta\tau$ can be approximated using Hertz's theory of elastic impact, b) energy flux at the compact surface is uniform over the entire contact area and is constant for times less than $\Delta\tau$. These are fair assumptions since the Hertzian impact is only mildly perturbed by the presence of a typically small powder compact, which has a small area of contact. Figure 1 schematically represents two balls colliding on a powder compact disk of thickness t_0 and radius r_0. This radius can be approximated as the flatened contact radius of the colliding balls, which are considered to undergo elastic collision. The kinetic energy is expended in elastically deforming the balls and plastically deforming the powder compact. The total kinetic energy of each ball is $E=1/2\ mV^2$, where m is the mass and V is the relative velocity of the impacting balls. An analysis by Maurice and Courtney (11) showed that only a small fraction β of the available energy is utilized in the plastic deformation process. Thus, the expended plastic energy U_p, which is assumed to be totally converted to heat at the contact, is $U_p= \beta E$. An equivalent amount of heat Q is manifested at each contact zone.

As shown in Fig.2, we model the heat transfer process at the contact of the sphere as a heat flux at the rate of q_1 per unit time per unit area, over a small circular area of radius r_0, in a semi-infinite medium. This is a reasonable approximation because the contact area in a typical impact event is very small compared to the surface area of the impacting sphere. Starting at t=0, heat flux is considered to be supplied at a constant rate q_1 which is given as,

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

Here, it is assumed that a fraction δ of the heat generated flows into the compact and therefore, a fraction (1-δ) of the heat flows into the sphere. Q represents an average quantity arising from the total deformation process over a time interval of $\Delta\tau$. The contact temperature T_c at the end of impact is obtained as (12),

$$T_c = T_o + \frac{2q_1\sqrt{\alpha_s \Delta\tau}}{K_s}\left\{\frac{1}{\sqrt{\pi}} - \mathrm{ierfc}\frac{r_o}{2\sqrt{\alpha_s\Delta\tau}}\right\} \tag{2}$$

Here, α_s is the thermal diffusivity and K_s is the thermal conductivity of the ball material, respectively and T_o is the ambient temperature. The geometry of heat flow into the powder compact can be modelled as a one dimensional thin plate (Fig.3) with prescribed heat flux q_2 at the surface $x=t_o/2$, which is given as,

$$q_2 = \frac{\delta . Q}{\pi r_o^2 \Delta\tau} \tag{3}$$

Due to symmetry of the problem, no heat flows across the mid plane. For the sake of simplicity, we ignore the temperature loss from the free ends of the compact, which however should be small because of a typically high aspect ratio of $2r_o/t_o$. Solving for the temperature distribution at the end of impact, we get,

$$T(x) = T_o + \frac{2q_2\Delta\tau}{\rho c_p t_o} + \frac{q_2 t_o}{2K_c}\left\{\frac{12x^2 - t_o^2}{6t_o^2} - \frac{2}{\pi^2}\sum_{n=1}^{\infty}\frac{(-1)^n}{n^2}\exp\left(-\frac{4n^2\pi^2\alpha_c\Delta\tau}{t_o^2}\right).\cos\left(\frac{2n\pi x}{t_o}\right)\right\} \tag{4}$$

Here, the subscript c denotes quantities related to the compact material. Thus, we get the contact temperature at $x=t_o/2$ as,

$$T_c = T_o + \frac{2q_2\Delta\tau}{\rho c_p t_o} + \frac{q_2 t_o}{2K_c}\left\{\frac{1}{3} - \frac{2}{\pi^2}\sum_{n=1}^{\infty}\frac{(-1)^n}{n^2}\exp\left(-\frac{4n^2\pi^2\alpha_c\Delta\tau}{t_o^2}\right).\cos(n\pi)\right\} \tag{5}$$

Because of temperature continuity, the contact temperature given by Eqs. 2 and 5 must be same. Thus,

$$\frac{2q_1\sqrt{\alpha_s\Delta\tau}}{K_s}\left\{\frac{1}{\sqrt{\pi}} - \mathrm{ierfc}\frac{r_o}{2\sqrt{\alpha_s\Delta\tau}}\right\} = \frac{2q_2\Delta\tau}{\rho c_p t_o} + \frac{q_2 t_o}{2K_c}\left\{\frac{1}{3} - \frac{2}{\pi^2}\sum_{n=1}^{\infty}\frac{(-1)^n}{n^2}.\exp\left(-\frac{4n^2\pi^2\alpha_c\Delta\tau}{t_o^2}\right).\cos(n\pi)\right\} \tag{6}$$

The fraction δ for the heat sharing between the compact and the sphere can be obtained from Eq.6. Then the temperature profile in the compact is determined from Eq.4.

So far we have analyzed the temperature increase of an impacted powder compact by considering the collision process as a discrete event and by considering the part of impact energy causing plastic deformation to act as a constant heat flux condition during a finite impact time $\Delta\tau$. Let us now turn our attention to an alternate approach where the heat flux caused by the dissipated plastic energy is considered to be acting instantaneously at time t=0, at the contact surface. In this case we ignore the presence of the thin powder compact and model the system as though there is an instantaneous plane source of radius r_o in the plane z=0 at t=0 (Fig.4). In this case, the contact temperature T_c at the end of impact is given as (12),

$$T_c = \frac{Q}{2\pi r_o^2 \rho_s c_{ps}\sqrt{\pi\alpha_s\Delta\tau}}\left\{1-\exp(-\frac{r_o^2}{4\alpha_s\Delta\tau})\right\} \quad (7)$$

where, ρ_s and c_{ps} are the density and specific heat of the ball material, respectively. The above Eqns. 5 and 6, or 7 provide an estimate of the contact temperature after an impact.

b) Cooling of the powder compact

Due to the statistical nature of powder impacts, it is expected that a compact, after undergoing an impact event, will undergo a free period before seeing another impact event. During this interval, it will disspate its heat to the surrounding medium. To estimate the time required for such a compact to cool down to the ambient temperature (T_o), we model it as shown in Fig.5, with heat being transmitted to the mill medium at the ambient temperature. The initial temperature f(x) is now considered to be the temperature T(x) (from Eq.4) just at the end of impact. The temperature at any time "t" during this cooling period is then given by,

$$T(x,t) - T_o = 4\sum_{n=1}^{\infty} e^{-\alpha_s\lambda_n^2 t}\left(\frac{\left\{h^2/K_s^2+\lambda_n^2\right\}\cos\lambda_n x}{\left\{h^2/K_s^2+\lambda_n^2\right\}t_o+2h/K_s}\right)\int_o^l f(x)\cos\lambda_n x.dx \quad (8)$$

where, λ_n's are obtained from the transcendental equation, $\lambda_n\tan(\lambda_n t_o/2) = h/k_s$, and h is the coefficient of heat transfer from the compact surface to the surrounding medium.

Results and Discussion

We first apply our present formulation to the experimental data obtained by Miller et al. (13), who utilized infrared measurements to study temperature rise due to an impact. They performed vertical drop-load experiments with 0.5 Kg mass on NaCl single crystal (approximately 2.45 mm x 2.45 mm x 1.5 mm), weighing 0.2 mg, placed on a saphire anvil. The terminal velocity at the moment of impact was estimated to be 18.5 m/s. Their results indicated that infrared emissions occur in NaCl, and also in several other crystalline and polymeric materials, to within a few microseconds after the imapact begins, indicating a sharp rise in temperature. The duration of impact event and the maximum temperature rise for NaCl measured by an infrared sensor, were estimated to be about 30 μs and 550 °C, respectively. For our calculation, we use the thermal properties (14) of NaCl as, α_s=4x10^{-6} m^2/s, C_{ps}=840 J/kgK and ρ_s=2150 kg/m^3. The energy sharing factor δ was found to be 0.18. It is known that NaCl undergoes little plastic deformation compared to metals. Maurice and Courtney (11) have tabulated values of the order of 0.005, as the fractional value for plastic deformation energy of aluminum, compared to elastic impact energy. Hence, in this case we can expect that even a smaller fraction of impacting energy will be used for plastic deformation of the NaCl crystal. Therefore, assuming a value of β to be 0.002, we obtain the contact temperature to be 670 °C. This is reasonable when compared to the actual measured value of 550 °C.

As a representative parametric calculation, we consider the grinding of niobium powder by stainless steel balls (8 mm diameter), moving with a linear relative velocity of 6 m/s. Without considering a rigorous calculation of plastic deformation energy, we consider two different reasonable values of β. The duration of impact $\Delta\tau$ and the contact radius r_o were calculated following Hertzian analysis and is given as (11),

$$\Delta\tau = 2.787 V^{-0.2}\left(\frac{\rho_s}{E}\right)^{0.4} R \quad (9)$$

$$r_o = 0.9731V^{0.4}\left(\frac{\rho_s}{E}\right)^{0.2} R \tag{10}$$

where, E and R are the Young's modulus and radius of the balls, respectively. The appropriate thermal properties of niobium powder and stainless steel balls are given in Table 1. The computed contact temperatures based on these values are given in Table 2. The calculated contact temperatures from the present formulation are substantially higher than the values of bulk temperature rise obtained by using the methods of Schwarz and Koch (8) or Maurice and Courtney (11), under similar conditions.

To estimate an upper bound to the contact temperature of this niobium compact by the alternate analysis (Eq.7), we obtain an increase in T_c to be 1260 ^oC for β=0.09 and V=6 m/s. As expected, this value is higher than 668 ^oC, calculated by using Eq.5, where we consider both the powder and the balls. It is also of interest to look at the actual temperature profile in the powder compact after a collision event. Figure 6 represents a plot of T(x) for the case where T_c is 668 ^oC. The resulting temperature is localized in areas close to the two contact surfaces. Miller et al. (13) also concluded to the similar effect in their experimental impact studies of various materials.

We now consider that a powder compact, during the interval between two subsequent impacts, travels alone at the same average velocity as the balls. Thus, for the present case of niobium (in air, for example), we obtain a Reynolds number of 40 ($Re=\rho_a t_o V/\mu$), where, ρ_a and μ are the density and viscosity of air, respectively. This gives rise to a Nusselt number of 2.1 ($Nu=0.234Re^{0.6}$). From this the heat transfer coefficient h is found to be 3.4 x 10^5 J/m^2.K.s. With these values we calculate the various roots λ_n's and the time for the contact temperature (T_c) to cool down to within 1 ^oC of its initial ambient value of 100 ^oC is found to be 4 x 10^{-3} s. Since the actual interval between two subsequent collisions is usually much longer than this value, we can conclude that the compact temperature will come down to its ambient value before undergoing another impact.

Conclusions

We have analyzed the temperature rise during an impact event of two balls colliding against a powder compact, which is the basic event in mechanical alloying. All of our calculations are based on head-on impacts, and hence, represent upper bounds to the possible temperature rise in a collision event. The calculations show that it is possible to have substantial increase in contact temperatures and hence, it can have considerable effect on the thermally activated mechanisms in mechanical alloying, such as, diffusion, etc. The analysis also indicates that the increases in temperatures are primarily localized near the contact regions. The model and its analysis have been applied to the results of impact experiments and are shown to provide meaningful correlation.

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TABLE 1
Thermo-physical Properties

	Niobium Powder	Stainless Steel Balls
Thermal Conductivity (K) J/m.s.K	57	16.2
Specific Heat (c_p) J/kg. K	275	50
Density (ρ) kg/m^3	8570	8000

TABLE 2
Computed Values of Contact T emperatures

Powder compact thickness = 10^{-4} m
Powder compact radius = 2.63 x 10^{-4} m

	T_c - T_o	
	V=6 m/s	V=8 m/s
β=0.03	223°C	396°C
β=0.09	668°C	1187°C

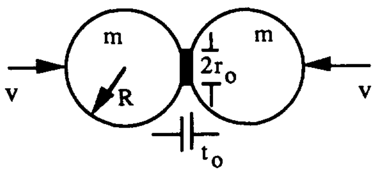

FIG.1 - Geometric parameters involving an impact between powder compact and two balls.

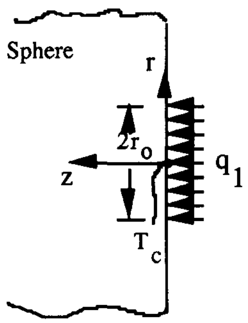

FIG.2 - Approximation of the balls as a semi-infinite medium with constant heat flux condition at a localized area.

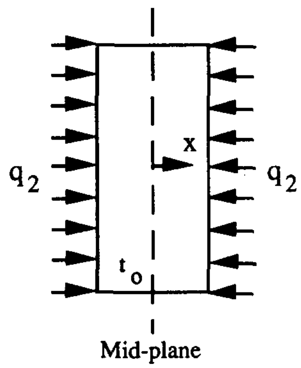

FIG.3 - Approximation of the powder compact as a semi-infinite medium with heat flux conditions at the two impacting surfaces

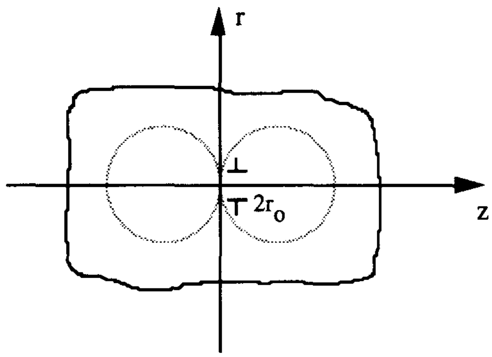

FIG.4 - Approximation of the impact event as an infinite medium with an instantaneous cylindrical surface source at the origin

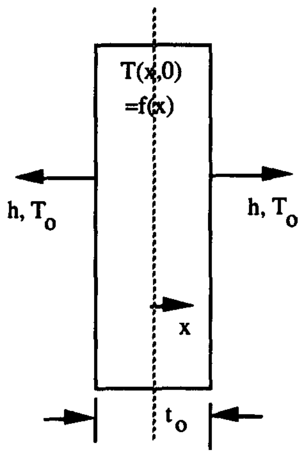

FIG.5 - Dissipation of heat from the powder compact surface during the interval between two impact events.

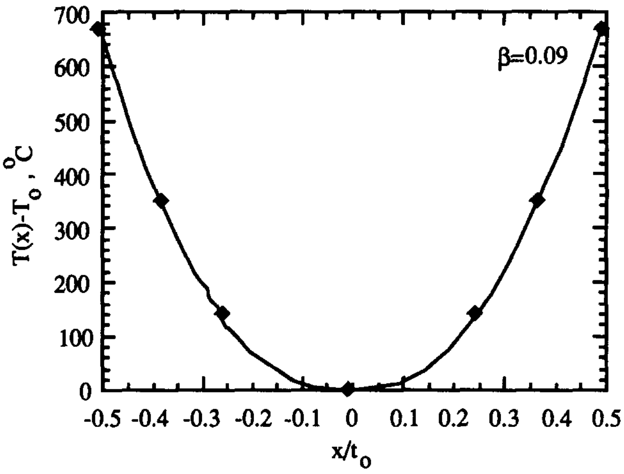

FIG.6 - A typical temperature profile T(x) across a powder compact thickness impacted with a velocity of V=6m/s.