Estimation of entrapped powder temperature during mechanical alloying

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Abstract

A simplified model was developed to determine the temperature of the powder particles at the point of collision during mechanical alloying (MA). The model showed that the temperature reached a maximum of ~473 K within 4–6 h of MA of a ternary blend of Al35Ni35Fe30 with the formation of AlNi phase.

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1. Introduction

The phase formation/transformation behavior during mechanical alloying (MA) has been a subject of significant interest for the past few decades. The mechanically activated alloying during MA, which is a solid state route carried out by high-energy ball milling, often involves complex mechanisms. Several factors are believed to influence the overall process, which include the free energy of the system [1–3], nano grain formation and/or defect induced disorder of the as-milled products [3]. A correlation between liquidus temperature and alloying kinetics was established by Pabi et al. [4]. In addition, the temperature rise accompanying heavy plastic deformation during MA is expected to play a major role in determining the kinetics of alloying and the nature of the final products as it directly alters the diffusivity and recovery of defects. Unfortunately, the dynamic nature of the ball milling process precludes direct measurement of the transient temperature at the ball–powder interface during milling.

Due to difficulties in direct temperature estimation during MA, considerable effort on modeling and other indirect methods have been applied to ascertain the possible temperature rise [5]. These models are guided by various approaches and assumptions [6–13] and there is a wide variation in the predicted temperature rise. For example, the Schwarz and Koch model [6] estimates a rise in the temperature by 321 K while the model by Bhattacharya and Arzt [12] arrives at a temperature as high as 621 K at identical velocity of the grinding ball. Work by Kwon et al. [14] demonstrated that the ball diameter as well as the presence of powder coating on the grinding balls and the vial wall during milling has a significant influence on the ball temperature during MA. However, their work did not consider the actual deformation of the ball surface due to collision and fails to quantify the influence of the thickness of the coating formed on the grinding ball surface on the temperature build-up.

Indirect experimental evidence based on the tempering effects observed during ball milling of Fe–1.2wt.%C martensite indicated a maximum temperature of ~538–548 K at the point of collision [7]. Studies revealed that there is wide difference in the experimentally determined values of temperature build-up at the contact point depending on the characteristics of the material subjected to milling [15]. Thus, it is clear that the estimation of the milling temperature is based either on entirely theoretical calculations or indirect means by monitoring specific reaction set that is applicable only for a particular system. Therefore, the development of a simplified technique that would estimate the temperature at ball–powder–ball/vial wall interface as accurately as possible...
is essential. The present work is an effort in this direction, which takes into account the experimentally determined global temperature rise of the system and the influence of the cold welded coating on the grinding balls/vial wall.

2. Experimental details

MA of elemental Al$_{35}$Ni$_{35}$Fe$_{30}$ powder blend was performed by high-energy ball milling using Fritsch P-5 planetary mill. Milling was carried out under a toluene bath in cemented carbide (CC) vials with CC grinding balls of 10 mm diameter. A disc speed of 300 rpm and a ball-to-powder weight ratio of 10 were used for MA. The vials were air cooled by forced air draft. The products were characterized by X-ray diffractometry using a Philips 1710 diffractometer. A highly sensitive digital thermometer (sensitivity of 0.01 K) was employed for the determination of bath temperature after every 1 h of milling. The tip of thermometer was inserted in the milling bath within 60 s of milling halt. It may be noted that a similar work [14] reported insignificant change in the bath temperature within the initial short period of milling halt.

3. A model for temperature effect

The existing models predict an adiabatic temperature based on energy transfer entirely by collision model, as the incorporation of a frictional constituent is always complex. Consequently, these models often lead to incorrect values. On the other hand, the present design of the high-energy planetary ball mills that are employed for the MA process, ensures a dual mode of energy transfer involving a considerable fraction of frictional contribution apart from the impact mode [16]. In order to overcome this problem, a highly simplified model is proposed to determine the temperature generated in the powder entrapped between colliding balls. As in other works, the present model adopts the collision theory. Simultaneously, it also makes use of the measured bath temperature, which is directly influenced by the total heat generated in the process due to impact and friction, as well as the heat loss owing to air-cooling of the vials. The following assumptions were made in the model:

(a) The kinetic energy of the grinding balls before collision is converted to heat energy during ball–powder–ball/vial wall impacts.
(b) Collision is of a Hertzian nature.
(c) Heat dissipation occurs through the vial wall.
(d) Some fraction of the heat is expended in heating up of the milling medium.
(e) The bath temperature acquires a stable temperature during each intermittent milling step of 1 h.

It may be noted that assumption (a) made in the present model considers the conversion of the entire kinetic energy of the grinding balls into heat energy. However, in real terms, a fraction of the total energy is also spent in inducing other changes in the system, for example, the generation of extra grain boundary area for nanocrystallite formation or phase formation/ transformation. Therefore, it is envisaged that the temperature predicted by the present model would be on the higher side of the actual temperature. In addition, earlier direct observation of the ball motion in planetary ball mills has shown that only a fraction of the collisions are of head-on type. It is expected that the fraction of head-on collisions will decrease with an increase in the extent of vial-filling due to its influence on the mean free path of the ball trajectory. This factor has been taken care-of in a subsequent section by the introduction of a vial-filling factor in the collision frequency calculation.

The model considers a simple heat transfer problem wherein the powder particle, trapped in each collision, gains thermal energy and attains a temperature of $T_C$, which is followed by heat dissipation to its environment comprising the grinding balls and milling media. This may be alternatively considered as equivalent to introducing a body of identical mass at temperature $T_C$ in a bath maintained at temperature $T_B$ ($T_C > T_B$) (Fig. 1). The heat loss through the vial wall occurs following Fourier’s theory of heat transfer [17] with the temperature on the outer wall assumed to be at room temperature ($T_{RT}$) as it is cooled by air draft. Thus, the heat balance equation becomes:

$$Q_1 = Q_2 + Q_3$$

where $Q_1$ = heat source (entrapped powder particles with heat energy acquired from the kinetic energy of the high velocity grinding balls)

$$Q_1 = fm_pC_p(T_C - T_B)$$

$Q_2$ = heat stored in the grinding medium

$$= (n_b m_b C_{pb} + m_p C_p + m_T C_{pt})(T_B - T_{RT})$$

where $f$ = frequency of collisions; $C_{pT}$, $C_{pb}$ and $C_{pt}$ are the specific heat of powder, ball material and toluene,

![Fig. 1. Schematic of the model with equivalent mass at temperature, $T_C$, in a bath at temperature, $T_B$.](image-url)
respectively; \( m_{pi}, m_h, m_p, m_T \) are the mass of powder trapped in each collision, mass of each ball, total mass of powder charge and the mass of toluene, respectively; \( n_b \) is the total number of balls.

while,

\[
Q_3 = \text{heat loss from the vial wall} = \frac{(T_B - T_{RT})}{\frac{1}{2} \pi ^2 \ln \left( \frac{r_2}{r_1} \right)}
\]

where, \( k \) = thermal conductivity of vial wall material; \( L \) = height of the vial wall; \( r_1 \) and \( r_2 \) are the inner and outer radii of the vial, respectively.

According to Hertzian collision theory, for head-on collision between two balls/ball and vial wall, there is deformation at the point of contact with the radius of deformed area given by [18]:

\[
R = \frac{0.8394 V_b^{1/5} m_b^{1/5} d_b^{2/5}}{E^{1/5}}
\]

where, \( E = \) Young’s modulus, \( d_b = \) ball diameter and \( V_b = \) linear velocity of ball. The collision frequency, \( f \), \( \text{s}^{-1} \) may be obtained from the expression [19]:

\[
f = \frac{K(\Omega - w)}{2 \pi 60 n_b}
\]

where, \( \Omega \) and \( w \) are the rotational velocities of the base plate and milling vials, respectively. \( K \) is the product of the factors \( K_1 \) and \( K_2 \) where \( K_1 \) is related to the time necessary for the dissipation of energy and has been shown to be \( \sim 1 \) while \( K_2 \) is the vial-filling factor as defined in [20], which is expected to reduce the mean free path of the balls and influences the ball trajectory and consequently accounts for the fraction of head-on collisions. The reduction in the velocity of the ball is also taken care-of by multiplying the ball velocity with the square root of the filling factor since the kinetic energy of the ball is proportional to the square of the impact velocity [21]. The mass of particles trapped during each ball–powder–ball/vial wall impact is given by:

\[
m_{pl} = 2 n R^2 \sigma.
\]

Where, \( \sigma \) is surface density of powder on the ball/vial wall. Considering the heat balance equation (Eq. (1)), it may be shown that:

\[
T_C = T_B + (T_B - T_{RT}) \left[ \frac{1}{f m_{pi} C_p} \left( \frac{2 \pi k l}{\ln \left( \frac{r_2}{r_1} \right)} + \frac{n_b m_b C_{ph}}{m_p C_p + m_t C_{ps}} \right) \right]
\]

The above equation indicates that for a measured bath temperature \( T_B \), the entrapped powder temperature at the point of ball–powder–ball collision, \( T_C \), may be calculated if \( \sigma \) is known.

4. A case study

The performance of the above model was evaluated by estimating the temperature generated during NiAl synthesis by MA of a ternary blend of Al\(_{35}\)Ni\(_{35}\)Fe\(_{30}\). Earlier work [22] revealed that a highly disordered AlNi phase is produced during MA of equiatomic blend of Al–Ni with ternary additions of Fe/Cr beyond 16 at.%, and the reaction occurs by a continuous diffusive mixing mechanism once the crystallite sizes of the ingredients reaches a critical nanocrystalline state. Fig. 2 shows the evolution of AlNi phase in the XRD patterns of the ball milled elemental blend. Studies [23,24] have shown that the initiation of AlNi phase from binary Al–Ni blends could be highly exothermic and therefore, a rise in temperature is expected during the phase formation.

Table 1 shows projected values of \( T_C \) at different \( \sigma \) for the typical range of bath temperatures observed during MA at a milling speed, \( \Omega, \) of 300 rpm. The table indicates that the temperature rise is related to the surface density of powder on the grinding balls (\( \sigma \)). Higher implies inelastic collision and leads to poor energy transfer and low heat generation. Fig. 3(a) shows the experimentally measured \( T_B \) during MA of Al\(_{35}\)Ni\(_{35}\)Fe\(_{30}\) at different milling stages. The data was transformed by the present model into temperature \( T_C \) of the entrapped powder. Fig. 3(b) shows the projected temperature rise at the collision point \( T_C \), as determined by the present model. It is worthwhile mentioning that even though \( \sigma \) should vary with the nature of the constituents, past studies [25] have indicated that it is quite realistic to assume a value of 0.3. It is evident from Fig. 3(a) and (b) that \( T_C \) reaches a maximum of \( \sim 473 \) K within \( \sim 6 \) h of milling, which incidentally coincides with the initiation
5. Conclusions

(1) A simplified model was developed to calculate the temperature of the as-milled powder at the collision point in the ball–powder–ball impact during MA, from the experimentally measured average vial bath temperature.

(2) The model estimates a maximum powder temperature of about 473 K during MA of AlNi from Al35Ni35Fe30 elemental blend. The powder temperature reached this maximum value within 6 h of MA, which triggered the AlNi phase formation.

References


Table 1
Calculated temperature rise at the point of ball–powder–ball collision for a given bath temperature, T_B, for various σ

<table>
<thead>
<tr>
<th>T_B (K)</th>
<th>T_C (K) at σ = 0.3</th>
<th>T_C (K) at σ = 1.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>313</td>
<td>363</td>
<td>328</td>
</tr>
<tr>
<td>318</td>
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<tr>
<td>338</td>
<td>471</td>
<td>378</td>
</tr>
</tbody>
</table>

Fig. 3. (a) The experimentally determined bath temperature during ball milling and (b) the projected temperature at the collision point estimated from the present model.

of AlNi(Fe) as determined from the XRD phase analysis of the milled product (Fig. 2). This possibly indicates that the extent of diffusivity at this temperature is quite adequate to trigger AlNi formation from the nanocrystalline ingredients.