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Mechanical alloying in a planetary ball mill: kinematic description

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ABSTRACT :

Based on a kinematic modeling of the planetary ball mill, the kinematic equations giving the velocity and the acceleration of a ball in a planetary ball mill apparatus are given. The kinetic energy transferred at the collision event and the shock frequency are also calculated. The confrontation of the calculation results to some experimental results documented in the material literature, shows that the end product depends on the shock power and not only on the kinetic energy.

The calculated shock powers correspond to three power levels :

- A low shock power level for which crystalline to amorphous phase transitions occur even at extended milling time.
- A medium shock power level for which a pure amorphous powder is formed.
- A high shock power for which a mixture of crystalline phase and an amorphous one will exist.

I. INTRODUCTION :

By ball milling pure elements as well as intermetallic compounds, an energy transfer from the milling tools to the milled powders is induced. The results of such a milling process are various : formation of amorphous phases by milling pure elements or by milling elemental metal ribbons, formation of intermetallics from pure elements, formation of powders having a fine microstructural scale, alloying of immiscible materials...[1]. Solid solution can also be considerably, supersaturated compared to the thermodynamic equilibrium [2]. The process is also inherently flexible. As such, it is reasonable to expect it to grow in importance. However, there are considerable gaps in the fundamental knowledge base relative to MA, as there has been little attempt to analyze it in a manner that would establish predictive capabilities for it.

In fact, N. Burgio et al. [3] do an attempt to correlate the milling operative parameters (the ball radius, the ball mass and the ball number) and the end product in a "Fritsch Pulverisette P 5" ball mill. D. R. Maurice and T. H. Courtney [4] try to give an approach defining the geometry and the basic mechanics of the powder-work piece interaction for several common devices used for MA, since these informations allow pertinent parameters of the process to be identified in terms of machine characteristics and process operating parameters.

In this paper we report on the results of a better geometrical description and on a complete formulation of the disc and vial absolute velocities and absolute accelerations for given disc and vial rotation speeds. The resulting kinetic energy, shock frequency and shock power are also reported. Then, we discuss some experimental results documented on the materials literature, reporting on the influence of the ball milling conditions on the milled end product.

II. THEORETICAL CALCULATIONS :

In this section, we report on the results of the kinematical study of the ball motion in the vial along one cycle. The details of such theoretical calculations are reported in our previous work [5]. Fig. 1 shows a modeling of a planetary ball mill, the amplitudes of the absolute velocity and absolute acceleration before the detachment event are respectively :

$$\|\vec{V}_a\|^2 = (R.\Omega)^2 + (r.w)^2 - 2.R.r.\Omega.w.\cos(\theta-\alpha) \tag{1}$$

$$\|\vec{\gamma}_a\|^2 = (R.\Omega^2)^2 + (r.w^2)^2 + 2.R.r.\Omega^2.w^2.\cos(\theta-\alpha). \tag{2}$$

Based on the fundamental dynamic principle, in a reference fixed to the ball, the detachment condition of the ball from the inner vial surface is :

$\cos(\alpha - \theta) = -r.w^2 / R.\Omega^2$. For more details, see ref.[5]. Thus, the amplitude of the absolute velocity and absolute acceleration at the detachment event, taking into account the ball radius are the following :

$$\|\vec{V}_a\|^2 = (R.\Omega)^2 + (r - r_b)^2.w^2.[1 + 2.w / \Omega] \tag{3}$$

$$\|\vec{\gamma}_a\|^2 = (R.\Omega^2)^2 - [(r - r_b).w^2]^2. \tag{4}$$

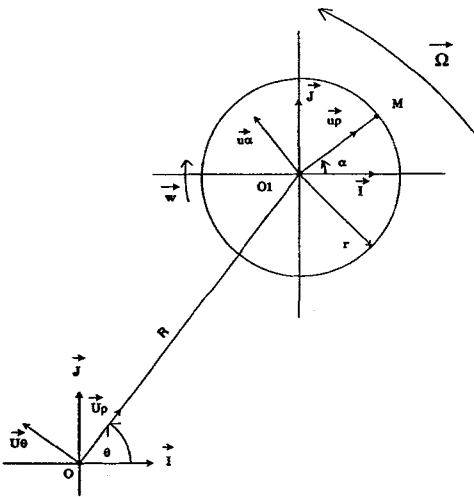


Figure 1 : Modeling of a planetary ball mill

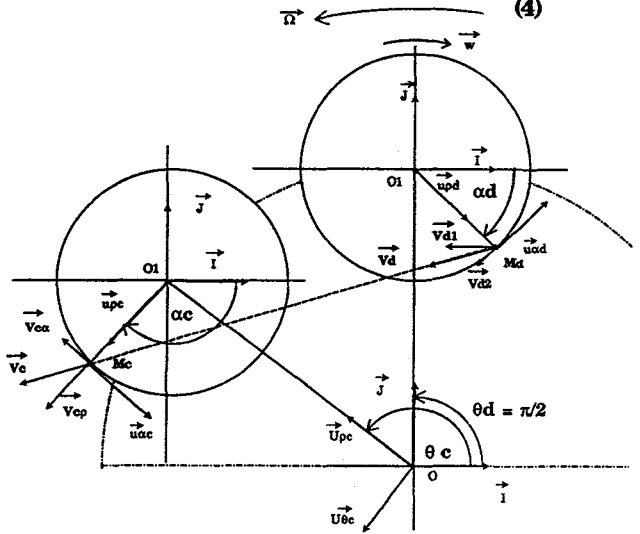


Figure 2 : Ball motion from the detachment event up to the collision one

To obtain the time between the detachment and the collision events, a numerical resolution using computer facilities is adopted. Fig. 2 shows the ball motion from the detachment event (supposed at $\theta = \pi/2$) up to the collision one.

The first collision event occurs when the following condition is fulfilled : $x = OP_x$ and $y = OP_y$, with x and y the ball coordinates after the detachment event and OP_x and OP_y the coordinates of a point of the inner vial surface. The calculation details of x , y , OP_x and OP_y are reported in ref. [5]. The resolution of this condition is done by the computer facilities. The numerical resolution consists to :

- 1) incrimination of the time value by a time step interval " Δt " of a microsecond,
- 2) calculation of the θ angle value,
- 3) variation of the α angle value from 0 up to -2π , by an incrimination of its value by a negative angle step interval $\Delta\alpha$ of -0.01 degree (the $\Delta\alpha$ value is negative to have a vial

rotation sense opposite to the disc one) and finally,
4) calculation of the OP_x and OP_y values and x and y values.

If the condition : $x = OP_x$ and $y = OP_y$ is fulfilled, we have the first collision point coordinates values (x and y) along the "X" axis and the "Y" axis as well as the time "t" needed between the first detachment event and the first collision event.

The kinetic energy " E_k " is given as :

$$E_k = 1/2.m.\|\vec{V}_d\|^2 = 1/2.m.\|\vec{V}_a\|^2. \quad (5)$$

The influence of the impact angle is also reported in ref. [5].

The shock frequency "f" is the number of collision per second. The cycle period is decomposed into two periods T_1 and T_2 with T_1 the period of time needed by the ball to go from the detachment point up to the collision point (the "t" period such as the condition $x = OP_x$ and $y = OP_y$ is fulfilled) and T_2 the period of time needed between the first collision event and the second detachment one. Thus, the shock frequency final expression is :

$$f = 1/T = 1/(T_1 + T_2). \quad (6)$$

When operating with a number of balls great than one, the shock frequency is equal to the product of one ball frequency reported above with the balls number corrected by a factor less or equal than 1. This fact is studied above by N. Burgio et al. [3].

The power released by the ball to the powders is the product of the frequency with the integral of the kinetic energy along one cycle period. It is given by the following expression :

$$P = f.E_k. \quad (7)$$

To have the total kinetic energy released from the ball to the powders during a ball milling duration "BMD", we will multiply the shock power (equation (7)) by the value of the ball milling duration.

III. RESULT AND DISCUSSION OF THE NUMERICAL CALCULATIONS :

Our calculations are carried on for the G7 planetary ball mill [6] which has the same disc radius than the so called Fritsch "Pulverisette 7". Such device allows the variation of the disc and vial rotation speeds independently.

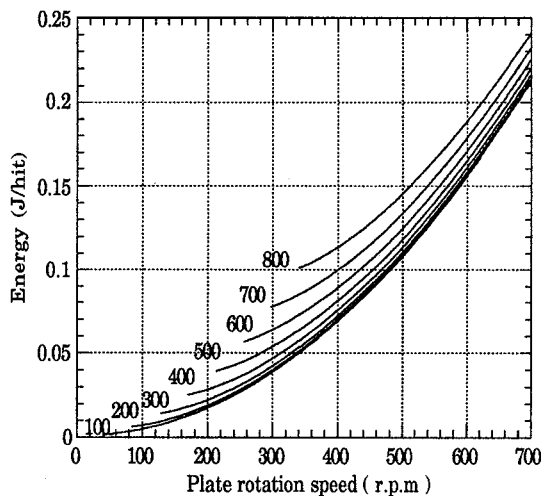


Figure 3 : Kinetic energy as function of the disc and vial rotation speeds (from [5])

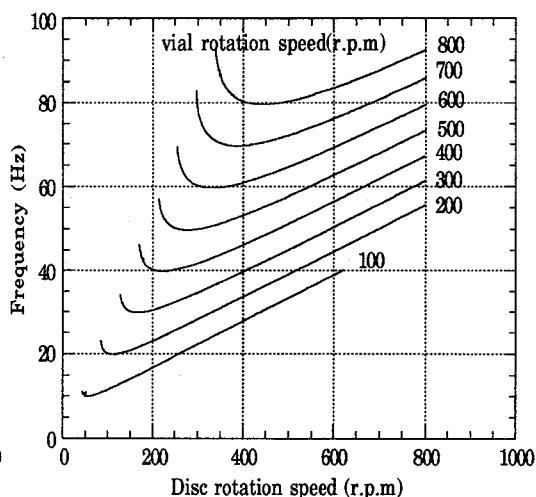


Figure 4 : Shock frequency as function of the disc and vial rotation speeds (from [5])

The so called G7 planetary ball mill has a disc radius equal to $75 \cdot 10^{-3}$ m. The vial radius is equal to $21 \cdot 10^{-3}$ m. The ball mass and ball radius are respectively equal to 14 g and $7.5 \cdot 10^{-3}$ m. 5 balls are used to calculate the shock energy, the shock frequency and the shock power. Fig. 3, 4 and 5, respectively give the kinetic energy released from one ball to the powders in one hit, the shock frequency and the shock power as a function of the disc and the vial rotation speeds.

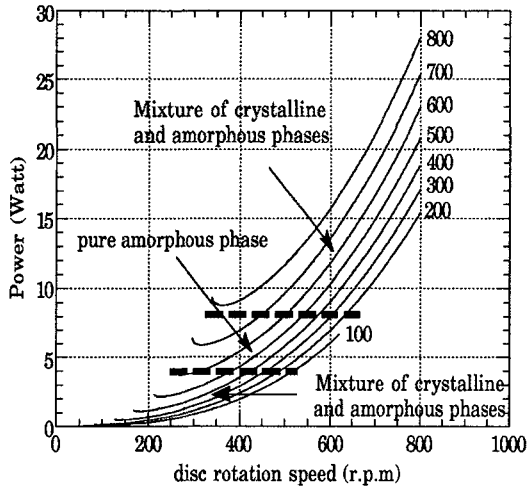


Figure 5 : Shock power as function of the disc and vial rotation speeds (from [5]).

Based on these above mentioned figures, the kinetic energy and the shock power increase as a function of the disc and vial rotation speeds. The shock frequency drastically decreases and then increases almost linearly as the disc rotation speed increases. For the so called G7 planetary ball mill, the maximum kinetic energy can reach 0.3 J/hit for disc and vial rotation speeds respectively equal to 800 and 800 r.p.m, the shock frequency and shock power can respectively reach 92.4 Hz and 28 W for the same ball milling condition.

IV. CONFRONTATION OF THE CALCULATION RESULTS WITH SOME DOCUMENTED EXPERIMENTAL RESULTS ON THE BALL MILLING PROCESS.

Based on the experimental results [6] and the calculated results, the amorphous phase formation is allowed for the shock power ranging from 4 W to 8.2 W. As the ball milling duration "BMD" used to obtain the amorphous phases is 48 hours [6], the total kinetic energy needed to obtain the amorphous phases will be the product of the shock power given by the ball milling duration. The same authors [6] report on the experimental ball milling conditions leading to the formation of a mixture of an amorphous and crystalline phases. Based on our calculation results, the ball milling conditions corresponding to the formation of a mixture of crystalline and amorphous phases correspond to two levels of power ; a low power level and a high power level. The low power level corresponds to the power values less than a minimum power value (4W) request to perform the crystalline to amorphous phase transitions. The high power level corresponds to the power values great than a maximum power value (8.2 W) request to perform the crystalline to amorphous phase transitions.

J. Eckert et al.[7] elaborate amorphous powders by mechanical alloying from Ni - Zr crystalline elemental powders. The MA was performed in a conventional planetary ball

mill (Fritsch "Pulverisette 5"). The used ball milling intensities are 3, 5 and 7. The authors [7] show that, for the ball milling intensity 5, a pure amorphous phase is formed and the ball milling duration needed to achieve the amorphization process was 60 hours. For the ball milling intensity 7, for the same ball milling duration (60 hours), the authors report on the formation of an intermetallic phase. For ball milling intensity 3, a ball milling duration of 60 hours was not sufficient for complete amorphization.

A very important point is that, the increase of the ball milling intensity [7] or the shock power [6] does not lead to the formation of only a single amorphous phase. In fact, at least, three situations may exist :

- For low shock powers, extended time is needed to have complete amorphization [7],
- For medium shock powers, a medium ball milling duration is sufficient to elaborate pure amorphous powders [6, 7],
- For high shock powers, for the same milling duration as for the medium shock powers, a mixture of intermetallic crystalline and amorphous phases [6] or intermetallic crystalline phases [7] is obtained.

It is assumed, at least, that a partial crystallization can occur during the mechanical alloying at high milling intensities and, the crystallization cannot simply be attributed to the milling but it must be an effect of excessive heating during the mechanical alloying [7]. Since the energy consumption increases when increasing the ball impact velocity and the coefficient of viscosity of the balls, which are assumed to be viscoelastic bodies, and, at least, the coefficient of viscosity is not a priori known [8], the estimation of the energy consumption and thus the resulting temperature increase within the powder particles is not precise. This fact does not agree with the conclusion of J. Eckert et al. [7].

In other hand, it was suggested that the critical defect concentration introduced by MA will promote spontaneous transformation to the amorphous state [9]. At this defect concentration, $G_c + \Delta G_d > G_a$, where G_c is the free energy of the crystalline phase, ΔG_d is the increase in the free energy due to the defects introduced by MA and G_a is the free energy of the amorphous phase. Consistent with this concept are the experimental observations [10] that intermetallic compounds with narrow homogeneity ranges tend to become amorphous during irradiation, while compounds with wide solubilities tend to remain crystalline. This difference was attributed [10] to a smaller increase in ΔG_d for a given defect density for the latter alloys, reflected by their ability to exist away from the perfect stoichiometry. This mechanism may explain the amorphization by MA when starting from crystalline powders of intermetallics. It does not seem adequate, however, to explain the amorphization by MA when starting from a mixture of pure crystalline powders. R. B. Schwarz et al. [11] suggest that the amorphization by MA when starting from a mixture of pure crystalline powders occurs by solid state interdiffusion reaction near clean boundaries between polycrystalline powders. The mixing is driven by the excess point and a lattice defects created by plastic deformations.

G. Martin et al. [12], assume that the frequency of forced jumps (in connection with the forced jumps induced by irradiation) scales with the shock power injected mechanically to the material. Indeed, most of the shock power is dissipated into heat, a small fraction (~ 10%) is injected into the lattice in the form of vacancies or antisites defects [13]. Following the above ideas, the authors [6, 14, 15, 16] do a systematic search for milling conditions which promote amorphization in a $Ni_{10}Zr_7$ compound. A narrow domain of amorphization is clearly visible. The authors [12], assume that amorphization proceeds below a certain power input and above a minimum energy per impact. It may be, if the power is too high, too large heat occurs.

Based on our calculated results and E. Gaffet et al. [6] experimental results, the ball milling conditions leading to the formation of the same amorphous phase, do not correspond neither to the same kinetic energy nor to the same shock frequency but almost

to the same shock power. Thus, we assume that only the released shock power governs the amorphous phase formation and the amorphization proceeds above a minimum power input and below a certain maximum power input.

Based on our calculation results and E. Gaffet et al.[6] experimental results, a dynamical end product phase diagram is mapped into three regions as a function of the shock power value : formation of a mixture of amorphous and crystalline phases reported for the low and high power values and formation of pure amorphous powders reported for the medium power values. Thus, we assume that, at low shock power values, the increase of the free energy of the crystalline powders, due to the increase of the concentration defect induced by plastic deformation is not too high to promote the formation of only a pure amorphous phase and the input crystalline powders are able to remain crystalline at even a such shock power. For the medium shock power values, $G_c + \Delta G_d > G_a$. Thus, only a pure amorphous phase is able to be formed. For the high shock power values, as like the low power level, the formation of a mixture of crystalline and amorphous powders occurs.

CONCLUSIONS :

Based on a kinetic modeling of the planetary ball mill, the kinematic equations giving the velocity and the acceleration of a ball in vial in a planetary ball mill are given. The kinetic energy transferred at the collision event and the shock frequency are also calculated. The confrontation of the calculation results to some experimental results documented in the material literature, show that the end product depends on the shock power, which is the product of the kinetic energy with the shock frequency, and not only on the kinetic energy.

Based on our calculation results and E. Gaffet et al.[6] experimental results, a dynamical end product phase diagram is mapped into three regions as a function of the shock power values : pure amorphous powders for the medium power values and mixture of amorphous and crystalline phases for low and high power values.

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