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PLASTIC DEFORMATION AND ITS INFLUENCE ON DIFFUSION PROCESS DURING MECHANICAL ALLOYING

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Introduction

Mechanical alloying is a process utilizing solid state diffusion reaction for producing powders with novel and unique properties. By this process, currently intermetallics (1, 2), amorphous materials (3, 4), metal matrix composites (5, 6) and dispersion strengthened alloys (7-9) are being produced.

While the processing related activities in mechanical alloying are extensive, except for a few notable attempts (10-12), relatively little has been done to model the fundamental processes in mechanical alloying. One of the basic mechanism governing mechanical alloying is believed to be solid state diffusion. In a recent paper (13), it has been proposed that diffusive reaction can be strongly affected by extensive cold working that accompanies mechanical alloying. The cold working generates increasing density of dislocations, which can enhance core diffusion process and also the resulting plastic deformation can dramatically affect the interfacial characteristics between powder particles by creating high concentration of vacancies and interstitials. Since the mobilities of interstitials are usually very high compared to vacancies, there may be a supersaturation of vacancies which can strongly affect the diffusion process. It is therefore important to have an understanding about the evolution of plastic deformation that takes place as the mechanical alloying process progresses in time. In this paper, we formulate a simple model, based on an analysis of high strain-rate deformation by Carroll and Holt (14), which can estimate the plastic deformation and the resulting dislocation densities, so one can analyze the diffusive process in mechanical alloying more accurately.

Model and Analysis

At the start of mechanical alloying process, a large number of particles (of the order of thousands) are trapped in a typical collision between two impacting balls. For the purpose of brevity in the rest of our paper, we call such an agglomeration a "powder compact". Schematically, such a compact, at the very beginning of the alloying process, is shown in Fig.1a. Subsequent impacts on this and other collections of compacts will continue to flatten the particles inside the compact as shown in Fig.1b. In our analysis, we simplify such a state of powder compact by a homogeneous medium (Fig.1c) containing a uniform distribution of pores. The pore sizes will continue to change with plastic deformation due to each impact event and it will also result in a change in the porosity. We make assumptions that, a) the pore distribution is statistically homogeneous and isotropic, b) pores are spatially isolated so that pore interactions are neglected, and c) initial porosity is known from some assumed stacking of particles. For our calculation, we consider an initial stacking sequence as shown in Fig.2. For this sequence, the pore size is obtained to be 0.46 times the average particle diameter and the porosity is 0.476. This particular arrangement has been assumed here as a matter of convenience, but any other arrangement could be used. Since the porosity changes considerably during the first impact itself, the subsequent results may not differ much from the results with the present assumption for the initial configuration.

Carroll and Holt (14) dealt with the constitutive relations for rate-dependent pore-collapse based on the properties of matrix materials and pore geometry. We assume that the hollow sphere model proposed by them is applicable in the present case, where the hollow sphere of the powder material has inner and outer radii such that the pore diameter and the overall porosity are those of the porous compact (Fig.1c). This is schematically shown in Fig.3. They concluded that the matrix incompressibility during pore collapse yields a good pore collapse relation for many materials. Neglecting any porosity change before the onset of plastic phase, they equated the rate of change of kinetic energy of the hollow sphere with the net difference between the rate of change of work by applied pressure p(t) and the rate of change in plastic work. In this way, the energy (χ_p) required per unit mass to reduce porosity from ϕ_o to ϕ is found to be,

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$$\chi_p = \frac{2Y(1-\phi)}{3\rho_s}\left[\ln\left\{\frac{\alpha_o^{\alpha_o}\,(\alpha-1)^{(\alpha-1)}}{\alpha^{\alpha}(\alpha_o-1)^{(\alpha_o-1)}}\right\}\right] \tag{1}$$

where $\alpha_o = 1/(1-\phi_o)$, $\alpha = 1/(1-\phi)$, the porosity ϕ is defind as the volume fraction of pore space, ρ_s the average solid density of the powder material, and Y is the flow stress of the matrix. The factor α_o is determined from the dimensions of the hollow sphere (Fig.3) and is given as,

$$\alpha_o = \frac{b_o^3}{b_o^3 - a_o^3} \tag{2}$$

Now, the plastic energy available in each impact is a small fraction of the available kinetic energy of the impacting balls. Approximate calculations by Maurice and Courtney (12) showed that this fraction (β) for various metals is in the range of very small values to about 0.1. Their calculation for elastic energy ignored the presence of the powder compact. A rigorous evaluation of the energy partitioning between the compact-balls elastic energy and the plastic energy for deforming the compact is a complicated issue, and we will take an empirical approach here. For a series of impacts on a particular porous powder compact, the elastic energy required for deformation will increase at each subsequent impact due to an increase in the elastic modulus of the compact. This increase in modulus occurs due to the decrease in porosity of the compact. Since the total impact energy can be assumed to be constant, the available energy for plastic deformation for a particular powder compact will decrease at each subsequent impact. The elastic energy (χ_e) of two impacting spheres has been calculated by Maurice and Courtney (12) using Hertz's analysis, and it is found to be proportional to $E_s^{0.2}$, where E_s is the Young's modulus of the spheres. To consider the effect of the porous powder compact in between the impacting balls, we can approximately modify this by considering an equivalent Young's modulus (E_{eq}) between the sphere material (E_s) and the porous compact material (E_c), which is expressed as,

$$E_{eq} = \frac{E_c E_s}{E_c + E_s} \tag{3}$$

The elastic energy will now be proportional to $E_{eq}^{0.2}$. In eq.3, E_c is expressed in terms of the well known Spriggs equation,

$$E_c = E_{co}\exp(-p.\phi) \tag{4}$$

where E_{co} is the Young's modulus of the compact material with zero porosity and p is a material constant. Thus, for all subsequent impacts on a particular compact, we calculate the available plastic energy χ_p by deducting the current elastic energy (χ_e) from the total available kinetic energy (χ) of the balls. Here, all energies are implied to be in Joules per unit mass (kg.) of the compact, Y in Pa. and ρ_s in kg/m^3.

Although Eq.1 was derived by Carroll and Holt for a material with constant flow stress, we consider the same equation to be applicable to each impact event, by assuming that during an impact the yield stress is strain rate independent, and that an average equivalent strain contributes to an increased flow stress Y, of the matrix, as,

$$Y = Y_o + H(\bar{\varepsilon}/2) \tag{5}$$

where Y_o is the flow stress of the matrix material at the beginning of an impact, H the linear hardening rate of the material and $\bar{\varepsilon}$ is the equivalent strain incurred during an impact event. Equation 1 is a simplified approximate dynamic pore-collapse relation by assuming that this hollow sphere response is the same throughout the material. Use of such a relationship to an impact event in mechanical alloying can be further substantiated by observing that the ratio between a typical compact thickness to ball diameter is very small and therefore, it can be assumed that the impact will create a uniform pressure at the surface of the compact. For the current impact event, $\bar{\varepsilon}$ is still an unknown quantity in eq.5. Noting that $b^3/a^3 = \alpha/(\alpha-1)$, $a_0^3/a^3 = (\alpha_0-1)/(\alpha-1)$, and neglecting any elastic strain, the average of the equivalent strain in the sphere is obtained as,

$$\bar{\varepsilon} = \frac{1}{3}\ln\left[\frac{\alpha(\alpha-1)}{(\alpha_0-1)^2}\right] \tag{6}$$

By substituting eqs.5 and 6 into eq.1, we obtain the average equivalent strain $\bar{\varepsilon}$ in the compact due to an impact event. Once the value of $\bar{\varepsilon}$ is determined, the new porosity level and flow stress at the end of impact is obtained from eqs.6 and 5, respectively, and these values are used as α_0 and Y_0, respectively, during the next impact event, assuming that the pores remain unchanged in size during elastic unloading at the end of an impact.

Plastic strain imparted on the powder compact due to repeated impacts creates an increased dislocation density inside the matrix material. The effective diffusivity D for mechanical alloying reaction can be strongly influenced by the total dislocation density ρ_L, and is given as (13, 15),

$$D = D_L.\exp\left(-\frac{Q_L}{RT}\right) + \beta b^2 \rho_L D_C.\exp\left(-\frac{Q_C}{RT}\right) \tag{7}$$

Here, D_L, D_C and Q_L, Q_C are the diffusion pre-exponent and activation energy of lattice and core diffusion, respectively, b is the Burgers vector, ρ_L is the total dislocation density and β is a core diffusivity factor. For evaluating the diffusion coefficient D, we can have an upper bound estimate of ρ_L by considering only statistical storage of dislocations but neglecting any loss of dislocations by dynamic recovery. Neglecting any dynamic recovery may be quite reasonable when one considers that the duration of a typical impact event is very short (order of 10^{-5} sec.). The rate of change of dislocation density with imparted strain is then given as (15),

$$\frac{d\rho_L}{d\varepsilon} = \frac{1}{100b}\sqrt{\rho_L} \tag{8}$$

Results and Discussion

Throughout the above formulation we considered the porous compact to have an average property representing various powder constitutents being alloyed. The compact is also assumed to statistically represent the whole powder in the mill. This way we have neglected the migration of powder particles to and from the compact. Also, the fracturing event has not been included, which means that the compact under consideration does not include a mixture of compact fragments with various states of deformation.

For the purpose of obtaining meaningful information from the present analysis we first define an energy input parameter Ψ as, $\Psi = \chi P_s / Y_i$, where Y_i is the average yield stress of the powder compact before any deformation takes place. Figure 4 shows the variation of a compact porosity with number of impacts. In the beginning the porosity quickly drops but as the number of impacts increases the rate of decrease in porosity considerably diminishes. This is clearly because the pores become more and more incompressible as their size is reduced. As intuitively expected, the rate of decrease in porosity increases as the energy input parameter Ψ increases. It should be noted here that through the variation in parameter Ψ, we include the effect of different compact size, the intensity of milling(ball diameter, velocity, mill geometry etc.), powder density and its initial average yield stress.

We calculate the plastic strain imparted in each impact and plot the evolution of dislocation density with increasing number of impact in Fig.5. In these calculations an initial state of the powder compact was assumed to contain a dislocation density of 10^{12} /m^2. Again, as the parameter Ψ increases, the rate of increase in the accumulation of dislocations increases. It is also observed that the dislocation density increases by a three order of magnitude for a relatively large mill intensity parameter Ψ. As an indication of the typical value of Ψ, for powders having an average yield stress of 100 Mpa and a density of 8 gm/cm^3, Ψ=0.6 can represent an attritor milling with ball velocity of 8 m/sec. With known values of mill operating parameters and powder properties, we can thus estimate the time-history of the average dislocation density ρ_L in the powder compact as the milling continues. However, it must be noted here that even though the parameter Ψ is a fully non-dimensional parameter, the plots presented here are not universal because the rate of work-hardening H enters into the calculation of porosity in an implicit way. Once the value of ρ_L is known at a particular time, the effective diffusion coefficient D governing the diffusion in the alloying process can be calculated from eq.7. An experimental study to verify the model prediction of the evolution of dislocation density developed here is currently under way.

Conclusions

This paper describes a simple model of the plastic deformation in a powder compact during mechanical alloying. The model utilizes the hollow sphere model proposed by Carroll and Holt and modifies it to describe deformation in mechanical alloying. The utility of the proposed model is that it avoids the complicacy of describing the powder deformation on a local scale by considering a mono-size distribution of pores present in between the deforming particles. A "Mill Intensity Parameter" Ψ is proposed which describes the simultaneous effect of mill intensity, powder compact size, powder density and its initial average yield stress.

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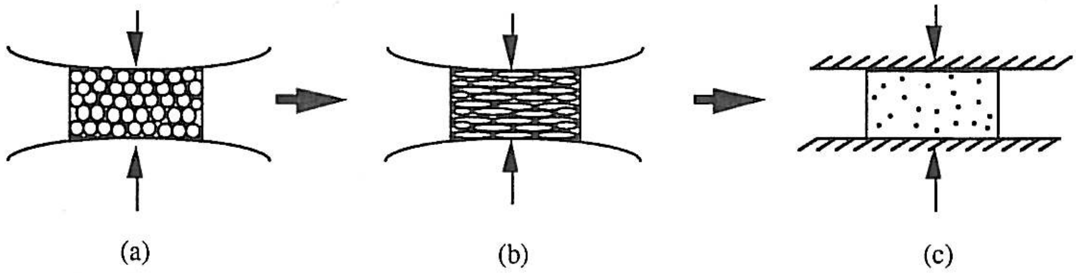

FIG.1 - Schematic representation of a compact consisting of many powder particles undergoing plastic deformation due to a series of impact events.

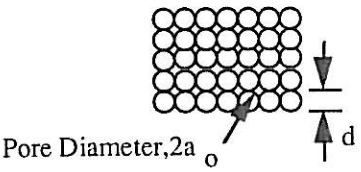

FIG.2 - Intial configuration of powder particles present in a compact at the start of first impact.

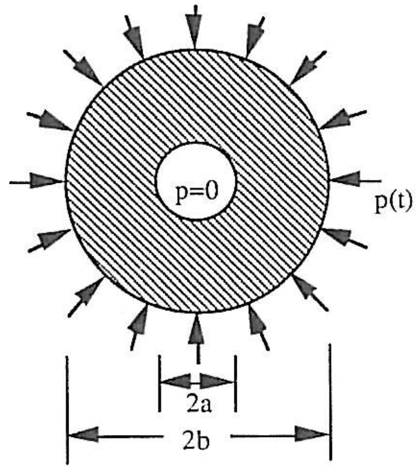

FIG.3 - Hollow sphere model describing the matrix material of the powder and a pore

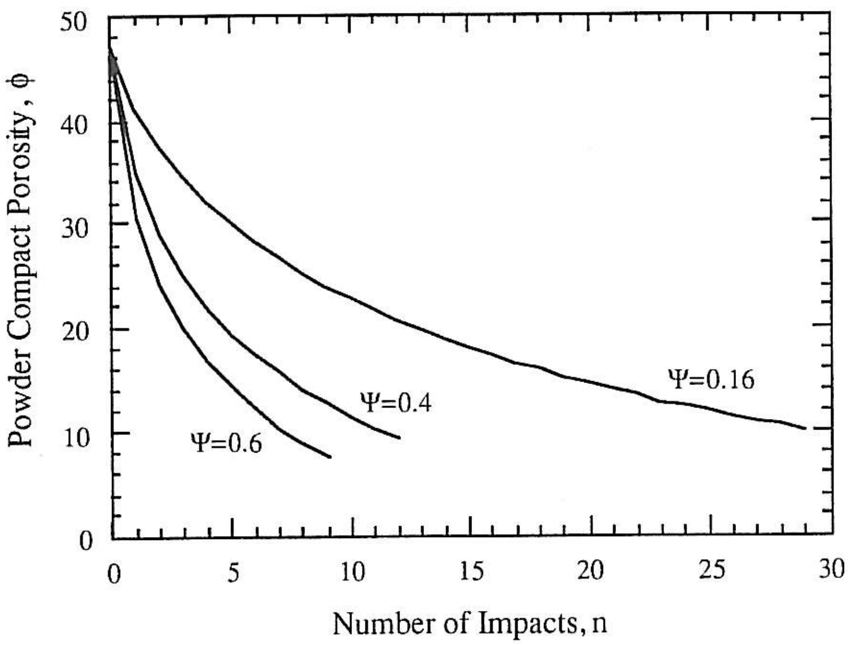

FIG.4 - Evolution of the compact porosity at various mill intensity parameter Ψ. The initial yield stress is assumed to be 100 MPa with a linear strain hardening rate of 300 Mpa. (assumed β=0.05 when the presence of the compact is ignored as in (12))

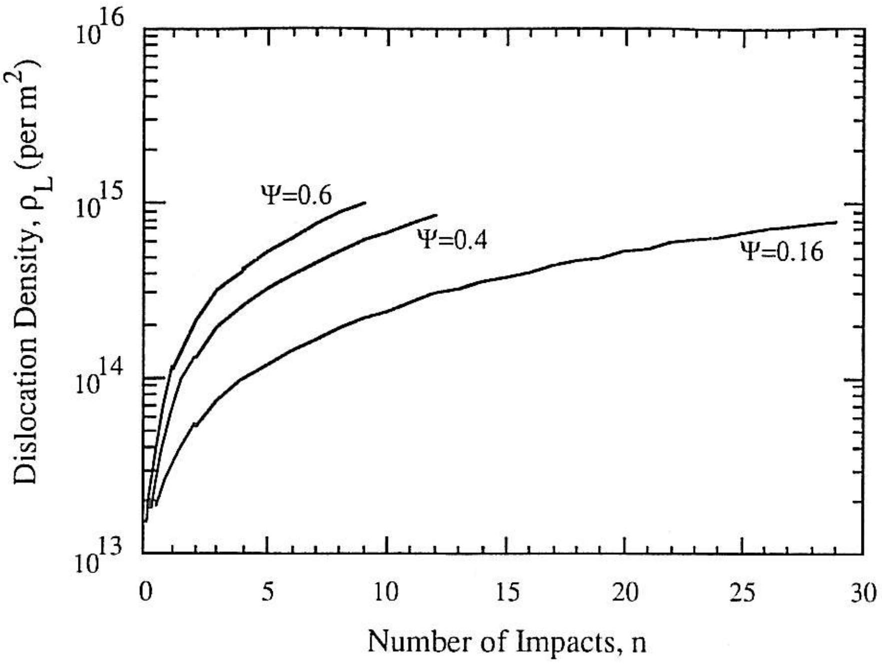

FIG.5 - Evolution of dislocation density with number of impacts at various mill intensity parameters. The initial dislocation density was assumed to be 10^{12} /m^2. (b=2.5×10^{-12} m)