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Mechanics and energetics modeling of ball-milled metal foil and particle structures

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ABSTRACT

The reported research establishes a semi-analytical computational predictive model of fractal microstructure in ball-milled metal foils and powder particulates, with emphasis on its transformation mechanics via an energy-based approach. The evolving structure is composed of reconfigurable warped ellipsoid material domains, subjected to collisions with the ball milling impactors following Brownian motion energetics. In the first step of the model, impacts are assumed to generate ideal Hertzian elastic stress fields, with associated bulk deformations quantified as per Castigliano's strain energy methods. In the second stage of the model, elastic energies are recast to produce frictional slip and plastic yield, thus resulting in surface micro-joints. Only two parameters of the model necessitate experimental calibration, performed by comparison of joint energy with laboratory tensile measurements on ball-milled multilayer Al-Ni foils. Model predictions of evolving internal microstructure are validated against SEM micrographs of Al-Ni powder particulate samples for different ball milling durations. Results demonstrate the capability of the model to accurately capture relevant fractal measures of the microstructure of ball-milled powders.

1. Introduction and prior work

Over the past three decades the materials community has made groundbreaking progress in mechano-chemistry research addressing *mechanical alloying* (MA) of metals and non-metallic materials. On the one hand, this has enabled a variety of transformative and impactful applications, as e.g. in *ball milling* (BM) fabrication of bimetallic and multi-material micro- and nano-structures, such as of nickel, iron and titanium aluminides etc., used for *self-propagating high-temperature synthesis* [1]. Such reactive metallic multilayers, upon thermal or electrical ignition, release heat, thus generating adiabatic temperatures of interest to metal joining, soldering and packaging applications [2]. More recently, planetary ball milling of Ni and Al powders in both high-energy (thermally transient) [3] and low-energy (thermally steady state) [4] implementation was experimentally researched. This showed promise for scalable manufacturing of self-similar (*fractal*) particles, ignitable in loose, cold-pressed pellet and sandwiched foil forms [5].

On the other hand, aside from its applications, influential intellectual motivation in MA originated from pioneering work performed through the 90's in establishing a conceptual framework and in numerical modeling of milling tool dynamics and microstructural evolution of BM particulates [6–9]. These investigations in planetary and vibratory milling elucidated fundamental aspects of BM kinematics and mechanochemistry of the alloyed materials in actual MA devices [7–10]. This seminal research inspired implementation of its basic principles,

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mathematical and experimental analysis in the context of planetary BM [11,12], horizontal rod mills [13] and BM energy transfer [14,15], eliciting considerable laboratory evidence and further theoretical refinement. Further effort tackled the kinetics of initial stages of MA [16,17], and recently structural refinement modeling [18,19] predicting evolution of lamellar thickness and grain size. Computational research addressed modeling of constitutive material behavior during impact for deformation analysis by *finite element methods*, as well as simulation of the ball dynamics, using the *discrete element method* [20]. Revived interest in MA culminated with recent comprehensive reviews [21], enabling new material design, analysis and optimization [2,5].

Computational modeling of MA has been facing the challenges of multi-domain, multi-scale, stochastic chaotic nature of the BM process. Despite valuable insights, however, numerical complexity of such an off-line simulation approach left an outstanding need for novel BM modeling tools with in-process computational efficiency, empowering real-time predictions of the spatially-distributed, time-evolving particulate structure. Such simulation tools would be advantageous as in-process MA *observers*, i.e. models running in parallel to the BM hardware and providing estimates of mechanically alloyed material states, such as particulate size and shape, structure and composition, and thermal and diffusive condition. Since these are usually inaccessible non-invasively and/or non-destructively in the enclosed, rotating BM setting, real-time model predictions could provide substitute feedback for closed-loop process control schemes. In addition, and beyond lamellar thickness, the full complex topology of material interfaces in the multi-scale, self-similar particulate structure needs to be captured by such modeling. This is because the fractal architecture directly determines the transport properties of MA products, and therefore their operational performance, such as in the case of ignitable reactive bimetallic systems [3,4].

A preliminary framework was recently proposed [22] towards such a real-time, experimentally validated computational simulation of the stochastic dynamics of the full fractal structure distribution in particulates during a BM process. Instead of numerically demanding discrete element methods for explicit BM kinematics, this approach adopts an analytical phenomenological probabilistic formulation of Brownian-like kinetics and energetics of impactor motion [23], matching computational predictions and laboratory measurements in the literature [24]. Analogous new stochastic descriptions of MA surface impact, contact, friction and volume deformation, coalescence and fragmentation mechanisms on universal geometric primitive elements of BM particle domains are also suggested. Instead of redundant vectorial and tensorial mechanics, material constitutive models are based on efficient scalar energy-based stress-strain transformations between ideal reversible and actual irreversible configurations. These are intended to preserve the fundamental underlying physics and chemistry of the chaotic BM process, and the concomitant fractal complexity of resulting particulate microstructures.

Thus, the objective of this article is to introduce and implement such novel primitive domain geometries and their energy-based transformations during the chaotic BM process dynamics, towards a real-time predictive simulation of the full fractal structure of MA particulates. The model description framework of a representative particulate composed of warped ellipsoid material domains (section 2.1) introduces a kinetic theory-based formulation of milling ball motion (section 2.2) for simulation of random collisions of the impactors (milling balls and vial walls). The model then departs with initially ideal elastic contact mechanics and energetics of the impact and joint locations of this particulate (section 2.3). These are subsequently recast to predict surface slip and dry friction (section 2.4), as well as plastic yield and strain-hardening of the materials (section 2.5), along with bulk deformation of the domains (section 2.6), generating heat and potentially micro-welded joints. Laboratory calibration of friction and yield parameters is performed experimentally by MA Al-Ni foils subjected to tensile lap testing (section 3.1). The composite model is validated by comparison of predicted microstructures of BM powders with experimental micrographs (section 3.2), with conclusions and suggestions for further work in section 4.

2. Model development

2.1. Model framework and assumptions

Morphological observation of ball-milled bimetallic particulate sections reveals a multi-scale self-similar microstructure (Fig. 1a) composed of lamellar network (*branching tree*) formations, which have evolved by deformation of globular agglomerates (*Apollonian packs*) of the original metal powders (Fig. 1b). This fractal microstructure transformation during the BM process can be described by the deformation and joining of these individual monometallic particle domains as *warped ellipsoid* (WE) primitives (Fig. 2). For direct comparison with experimental planar micrographs (e.g. Fig. 1a), the model only focuses on a 2D section of the particulate, whereby each WE is described, to a second order approximation, by only 8 scalar parameters: centroid coordinates X, Y; orientation angles ϕ_x, ϕ_y; semi-axes l_x, l_y; and curvature radii R_x, R_y (Fig. 2). This 2D geometric configuration results in computational efficiency of the model over a 3D formulation, which would require 21 parameters for each WE. At the same time, parametric self-similarity of the WEs is preserved as they reshape from spheroidal ($l_x \approx l_y$, $R_x \approx R_y$) to lamellar ($l_x \gg l_y$, $R_x \gg R_y$) form, resulting from interaction with impactors, i.e. the BM balls and vial walls, and other particles. The model actually carries out all computation below on extrapolated 3D domains, with semi-axis $l_z = \sqrt{l_x l_y}$ so that equal WE section areas correspond to equal domain volumes, and radius $R_z = 2R_xR_y/(R_x + R_y)$ leaving the equivalent local curvature of the section boundary invariant. Initial distributions of WE parameters are interpolated from contours of the initial ball-milled loose powders on actual micrographs.

During BM, the simulation tracks dynamic evolution over time of one representative particulate as it is progressively transformed by deformation of its WE domains, and as its joins with adjacent particles (WEs) and clusters (WE assemblies) over its boundary (Fig. 3). For this purpose, the model adopts a *Lagrangian* approach, following a moving *Cartesian* frame (x, y coordinate system) fixed with respect to the studied particulate. As in Fig. 3, the particulate is surrounded by an adjacent layer of randomly selected particles and clusters, and the assembly is impacted at a random location by BM balls and vial wall impactors, moving at incidence velocity v and orientation ϕ. The model ignores presence of the inert gas atmosphere in the vial, potential liquid process control agents, as well as gravitational and dynamic inertial effects. It also assumes steady-state thermal equilibrium in the vial and its contents (as e.g. in low-energy BM). In other words, isothermal process conditions are considered, neglecting the dependence of domain dimensions and material properties on thermal effects. In addition, material properties are evaluated for an average deformation rate of impact during BM, and strain rate effects are neglected. Absence of material transformations via diffusive and reactive phenomena at interfaces and bulk volumes during the BM process is also presumed.

All particulate materials are assumed homogeneous and isotropic with linear elasto-plastic behavior. In the material bulk, the constitutive behavior is described by a bilinear strain-hardening stress-strain (σ, ε) or (τ, γ) curve, at elastic moduli E,