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Full Length Article

Modeling of nanoparticle agglomeration and powder bed formation in microscale selective laser sintering systems

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ABSTRACT

Additive manufacturing (AM) has received a great deal of attention for the ability to produce three dimensional parts via laser heating. One recently proposed method of making microscale AM parts is through microscale selective laser sintering (μ-SLS) where nanoparticles replace the traditional powders used in standard SLS processes. However, there are many challenges to understanding the physics of the process at nanoscale as well as with conducting experiments at that scale; hence, modeling and computational simulations are vital to understand the sintering process physics. At the sub-micron (μm) level, the interaction between nanoparticles under high power laser heating raises additional near-field thermal issues such as thermal diffusivity, effective absorptivity, and extinction coefficients compared to larger scales. Thus, nanoparticle's distribution behavior and characteristic properties are very important to understanding the thermal analysis of nanoparticles in a μ-SLS process. This paper presents a discrete element modeling (DEM) study of how copper nanoparticles of given particle size distribution pack together in a μ-SLS powder bed. Initially, nanoparticles are distributed randomly into the bed domain with a random initial velocity vector and set boundary conditions. The particles are then allowed to move in discrete time steps until they reach a final steady state position, which creates the particle packing within the powder bed. The particles are subject to both gravitational and cohesive forces since cohesive forces become important at the nanoscale. A set of simulations was performed for different cases under both Gaussian and log-normal particle size distributions with different standard deviations. The results show that the cohesive interactions between nanoparticles has a great effect on both the size of the agglomerates and how densely the nanoparticles pack together within the agglomerates. In addition, this paper suggests a potential method to overcome the agglomeration effects in μ-SLS powder beds through the use of colloidal nanoparticle solutions that minimize the cohesive interactions between individual nanoparticles.

1. Introduction

Harnessing heat transfer at the nanoscale is essential for the development of microchips in semiconductors, micro/nanoelectronics, integrated circuits, and micro/nano electromechanical systems (MEM/NEMS) [1]. Today, using nanomaterials such as nanowires, carbon nanotubes, graphene, and metal nanoparticles is common in these types of systems. Nanomaterials are generally used in these systems because the thermal, optical, and electromechanical properties of nanomaterials are quite different from the properties of the bulk material and can be tuned by controlling the shape and size of the nanostructure [1]. The key fields where nanomaterials have recently been used in additive manufacturing technologies are microscale selective laser sintering (μ-SLS), three-dimensional (3D) printing, and stereolithography [2]. μ-SLS is a relatively new additive manufacturing technique in which the structures or objects are fabricated from the bottom up by adding materials layer upon layer [3]. In this technique, a laser that has been focused down to approximately 1 μm is used to sinter together nanoparticles in a designed pattern on each layer before the next layer of nanoparticles is added to the system. This process is then repeated until an entire 3D structure with microscale features is fabricated. Through the use of precise focusing objectives, ultrafast lasers, and nanoparticle based powder beds it is possible to achieve micron scale feature resolutions with this technique.

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μ-SLS has many advantages over other manufacturing techniques in terms of the flexibility, cost, and finishing quality. Furthermore, μ-SLS provides design freedom and has a lower level of waste and harmful chemicals. Using nanoparticles which can be synthesized with different shapes such as rods or spheres for microscale selective laser sintering can also significantly improve the sintering characteristics and the finishing quality of the parts [2]. However, models for nanoparticle interactions and powder bed generation with nanoparticles are not available for SLS at nanoscale. This is because nanoscale modeling offers many challenges; for instance, a continuum model which is used for micro and larger scales is no longer valid. Also, a ray tracing model cannot be used to obtain the extinction and effective absorption coefficient of a powder bed as the laser wavelength is greater than the characteristic length of the particles [4,5]. Hence, modeling the nanoscale powder bed with nanoparticles for SLS is quite different from modeling micro or larger scales. For example, cohesive forces, which are the sum of the attractive or repulsive intermolecular attractions between molecules, dominate interactions between the particles at nanoscale [6,7]. These cohesive interactions can create significant agglomeration effects in particle beds containing nanoscale powders which are not typically seen in SLS powder beds that contain only microscale powders. These agglomeration effects can significantly reduce the packing density of the particles in the powder bed which can result in significant voids in the final sintered part. Additionally, particle size distribution is another factor affecting the sintering process at the submicron level [8]. Most powder beds with nanoparticles have non-uniform size distributions which effect the sintering quality and overall shrinking of the parts produced. Hence, it is essential to model the particle–particle interaction at nanoscale accurately in order to understand the overall powder bed and size distribution effect on the selective laser sintering process. Therefore, in order to better understand the parameters that effect void formation in μ-SLS parts, this paper uses discrete element modeling techniques to investigate the role of cohesive forces and particle size distribution on the packing density of nanoparticles in a μ-SLS powder bed.

1.1. Background

Discrete element modeling (DEM) has been a commonly used method for examining the packing and agglomeration of particles in powder systems over the past 30 years. Early DEM based computational models focused on analyzing how microscale particles with uniform size distributions pack together in powders where gravity is the major driving force for packing [9,10]. In these microparticle based systems, cohesive forces such as the van der Waals force do not play a significant role in how particle systems pack together [11]. Instead, the size distribution of particles within the powder system is the most important factor in determining in how the particles pack together in these types of systems [12]. However, in nanoparticle based systems, cohesive forces do play a significant role in the agglomeration and packing of particles within the powder system [13]. Therefore, both cohesive forces as well as particle size distributions need to be considered when analyzing packing in nanoparticle based systems [14].

One of the most common methods for modeling cohesive forces in nanoparticle based systems is to use the Johnson, Kendall, Roberts (JKR) model [15]. In the JKR model of cohesive contact, a balance is created between the elastic energy stored in the particle and the loss in surface energy that is created when two particles are in contact. In the JKR model, only contact pressure and adhesion within the area of contact are considered. This model has been used to examine both how nanoparticles agglomerate and pack together within a powder [16] as well as to model the strength of those agglomerations [17,18].

Cohesive contact is modeled in this paper using an alternative to JKR theory called the Derjaguin-Muller-Toporov (DMT) model [19], which accounts for cohesive forces both within and outside the area of contact between the nanoparticles in order to help accurately model the agglomeration of nanoparticles within the μ-SLS powder bed. The DMT model is used in these simulations because DMT theory has been shown too accurately model metal and ceramic nanoparticle systems, such as the copper nanoparticle system analyzed in this paper [20]. This is because these systems tend to have relatively small and hard particles with low surface energies and, therefore, adhesion in these systems is dominated by weak, long-range attractive forces outside the contact zone [21–23]. In addition, nanoscale asperities on the surface of the nanoparticles can play a significant role in the cohesive forces effecting the nanoparticles [24,25]. Therefore, the DMT contact adhesion model used in this paper has been modified to account for the fact that nanoscale roughness on the surface of the nanoparticle can significantly affect the adhesion forces on the nanoparticles.

In this paper, modified DMT theory is used to examine both how different types of cohesive interactions (none, weak, and strong) and particle size distributions (log-normal, Gaussian, uniform) effect how powder beds form (including packing fraction and density) in microscale selective laser sintering systems. This paper also explores how the presence of a gravitational driving force effects particle packing within a nanoparticle based powder bed system. This includes examining both how all of these parameters effect the agglomeration of nanoparticles as well as the packing of nanoparticles within individual agglomerates. This type of study has not been previously performed in the literature and is very important for designing powder spreader systems for μ-SLS. In addition, the results of this study provide a key motivation for moving from a dry powder spreading mechanism to one involving solvents in nanoparticle based powder bed systems.

2. Modeling approach

The powder bed, consisting of solid, spherical nanoparticles that are generated by defining a position and radius, is created using the discrete element method (DEM) in a multiphase computational fluid dynamics, MFIX. Particle packings are generated using the MFIX-DEM discrete mass inlet function with each particle interacting with its neighboring particles. The particles are initially distributed randomly within the powder bed domain and are given an initial velocity and an initial set of boundary conditions. Forces such as gravitational and cohesive forces are also applied to each particle. Material properties such as diameter, density, and different particle size distribution can also be defined by the user. The MFIX-DEM approach is explained in detail in [26] and summarized briefly below. Our simulation analysis predicts different force analysis contributions such as cohesive and gravitational force within given particle distributions.

2.1. Discrete element method (DEM)

In the discrete element method (DEM), a number of spherical particles, N_m, with diameter, D_m, and density, ρ_{sm} are used to represent the nanoparticle in the powder bed. The total number of particles in the powder bed is given by the summation of each spherical particle over the total number of solid phases, M, as given by Eq. (1).

$$N = \sum_{m=1}^{M} N_m \tag{1}$$

Each of the N particles is defined within a Lagrangian reference at time t by its position, $X^{(i)}(t)$, linear velocity, $V^{(i)}(t)$, angular veloc-

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