Computational Materials Science 125 (2016) 255–262

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Shock wave sintering of Al/SiC metal matrix nano-composites: A molecular dynamics study

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ARTICLE INFO

Article history:
Received 21 January 2016
Received in revised form 17 August 2016
Accepted 21 August 2016

Keywords:
Metal Matrix Composites (MMCs)
Nano-structures
Sintering
Shock wave
Mechanical properties
Molecular dynamics

ABSTRACT

Mechanical properties of nano-composites produced by shock wave sintering of aluminum and silicon carbide nano-powders are investigated using Molecular Dynamics (MD) simulations. In this regard, the shock wave response of aluminum and silicon carbide nano-particles, arranged in a BCC super-lattice, is studied via the NPHug Hugoniostat method. Moreover, the effect of the initial hydrostatic compaction of powders as well as the cooling rate of the shocked material on the mechanical properties of the shock-sintered nano-composites is investigated. Employing the Hugoniot curves corresponding to the powders, it is concluded that an initial hydrostatic pressure, leads to a less temperature rise and higher shock wave velocity. Moreover, the uniaxial loading test simulation is utilized to determine the mechanical properties of the final products. It is illustrated that increasing the shock pressure leads to an enhancement in the mechanical properties as a result of the formation of fiber reinforced nano-composites. The initial pressure exerted on the nano-particles, however, results in weakening of the sintered nano-composite. Furthermore, it is shown that an appropriate cooling rate can result in the activation of the diffusion mechanism after the shock wave passage which is helpful in increasing the bonding strength of nano-particles.

1. Introduction

Consolidation of powders with the help of thermal energy, which usually happens at about 2/3 of the melting temperature, is called sintering. The main advantage of this process over other manufacturing methods are less energy consumption, high ability to get complex shapes, dimensional precision in final product, excellent surface finish, repeatability and high reliability. Thus, sintering is one of the most economical manufacturing processes, especially in mass production [1,2].

Metal Matrix Composites (MMC) are composed of a hard ceramic phase dispersed in a soft metallic matrix. This kind of structure has found applications in many areas of life. Due to difference between thermal expansion coefficient of metal matrix and ceramic reinforcement, poor wetability of ceramics and formation of brittle phases at higher temperatures, there are many problems in the production of parts out of MMCs [3]. Since sintering process benefits from lower temperature and diversity of powder from metal to ceramic, it can be used as the main process in manufacturing of MMCs.

Usually, the size of ceramic reinforcements in MMCs is in the range of micrometer. Micro-size ceramic particles provide MMCs with higher yield and Ultimate Tensile Strengths (UTS), but lower ductility with respect to the corresponding pure metal. Employing nano-size ceramic reinforcements in MMCs, one can maintain good ductility as well [4]. Besides, nano-size ceramic reinforcements can induce high temperature creep resistance and better fatigue life [3]. Nanoparticles have a higher level of activity with respect to their micro-size counterparts that make them suitable in this manufacturing process.

In the sintering process a kinetic energy should be imposed to the material to make local bonding between particles. This energy can be obtained by shock waves. Shock is a discontinuity in density, pressure and temperature which propagates into the material [5]. Although shock is a continuum concept, its length scales are very small and sometimes comparable to the lattice spacing of the material under study. The importance of considering the atomic behavior of the material in scrutinizing this phenomenon is highlighted by these small length scales [6,7]. Thus, the atomistic simulation method is an appropriate tool in studying shock behavior of materials.

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http://dx.doi.org/10.1016/j.commatsci.2016.08.032
0927-0256/

Shock wave sintering is a method in which powder compaction happens without any direct external heat sources thanks to the shock pressure. Plastic yielding is followed by powder densification. Besides the plastic yielding, localized heating via inter-particle friction during the shock wave propagation, facilitates local bonding between particles. In contrast to micro-size particles in which heating is superficial, for nano-particles heat transfers through the whole sample [8]. This relatively uniform heat transfer leads to a better bonding. So, it is worthwhile to study shock consolidation of nanoparticles.

Among all the atomistic simulation methods, MD simulation, due to its ability in modeling atomic interactions in nano-scale has met diverse applications. Tracing motion of all atoms with the aid of solving Newtonian equations of motion is the main idea of MD. In this scheme, the interacting forces between particles are obtained by using the interatomic potentials. Therefore, MD simulation is applied as a virtual laboratory without the shortcomings of the real experiments.

This approach has been utilized as the main tool in a wide range of investigations on the nano-scale sintering and shock wave. For instance, Alarifi et al. modeled the sintering process of silver nanoparticles [9]. They concluded that in the sintering of nanoparticles after a rapid neck formation at the beginning, there was a gradual increase in the neck radius followed by the final shrinkage. Moreover, Cheng and Ngan studied the intermediate structures formed during sintering of copper nano-particles [10]. They observed the formation of a variety of structures including single, double and triple twins during the process. Investigating the laser sintering process for different sizes of gold nanoparticles with the help of MD simulation, Yang et al. concluded that the stable neck width depends on the size of nanoparticles [11]. Tavakol et al. studied the sintering process of nano-particles through MD simulation and concluded that both of diffusion and plasticity are the main mechanisms of the process depending on the temperature and particle size [12]. In addition, Liu et al. studied the response of the tungsten to the shock loading using MD simulations. They concluded that the propagation of the shock wave is strongly dependent on the loading orientation in the tungsten crystal [13]. Employing the same simulation methodology, Lee et al. observed the movement of elastic, dislocation forming, elastic-plastic and phase transition waves in different shock loading velocities [14]. Stress wave consolidation of nano-particles is studied by Li et al. using the atomistic simulations [15].

Most of previous studies on the shock wave consolidation have shed light on the experimental approaches of the process. Kondo et al. experimentally investigated the shock compaction of silicon carbide powders [16]. They observed that disruptive effects of shock wave help developing the powder compacts with higher densities. Studying sintering of shock treated AlN powders, Miao et al. deduced that the residual strain at the crystalline structure is the driving force for the process [17].

Moreover, some researchers have employed the shock compression to obtain nano-powders owning especial properties. In 2000, Wu et al. sintered shock treated aluminum nitride powders [18]. They showed that sintering of shock treated powders led to a higher final density. Also, those dislocations which are introduced into the powders via shock wave enhanced the diffusion process by making new diffusion paths. In 2004, Lu et al. compared the sintering of normal Si_3N_4 powders with that of the shock treated ones [19]. They emphasized that shock treatment can increase the strength of sintering products more than 40%. Synthesizing Pb$(Zr_{0.95}Ti_{0.05})O$ powders with the aid of shock induced chemical reactions, Wang et al. described those lattice defects and distortions occurred by the shock wave passage, as the main cause of an increase in the sintering activity [20]. More sintering activity, subsequently, results in significant decrease in the sintering temperature.

The main goal of the present study is to investigate the shock wave sintering of Al and SiC nano-powders to produce Al/SiC nano-composites. Al matrix composites have applications in different industries due to their high operational temperature, elastic modulus, wear resistance, acoustic fatigue resistant and ability to work in gas, vacuum and radiation environment [21–23]. These structures, thanks to their lower coefficient of thermal expansion, lower density and higher thermal conductivity, are expected to be more competitive in electronic packaging [24, 25].

In this research, shock wave sintering of Al/SiC nano-composites is studied. The aim of the investigation is to illustrate the effect of parameters such as the shock pressure and the cooling rate on the mechanical properties of the shock sintered nano-composites. Since there are differences in the main mechanisms and final products of free and field assisted sintering, it is worthwhile to study the effect of initial powder compaction on the whole process [2]. To this end, the MD approach is utilized in calculating the Hugoniot curves and mechanical properties of nano-composites. By the way, all of the simulations are done using LAMMPS molecular dynamics software [26].

The current paper consists of four sections. After a brief introduction and literature review of the subject, the simulation method is described in the second section. The third section is devoted to presentation and discussion on the simulation results. The final section of the paper is dedicated to the concluding remarks.

2. Simulation method

2.1. Interatomic potentials

In MD simulations the interactions between atoms are calculated through the interatomic potential functions. Since in this work shock wave sintering of Al/SiC nano-composites is investigated, there is a need for proper potential functions for the interactions between aluminum atoms, silicon and carbon atoms in silicon carbide particles and aluminum with silicon carbide. So, the first step is to choose the proper interatomic potential functions.

In order to obtain the forces between aluminum atoms, the embedded atom method (EAM) potential is employed. The total energy of the EAM potential function can be approximated by:

$$E_{total} = \sum_i F_i(\rho_i) + \frac{1}{2}\sum_{i\neq j}\phi_{ij}(R_{ij}) \tag{1}$$

where ρ_i is the total electron density surrounding atom i due to the neighboring atoms, $F_i(\rho)$ is the energy which is needed to embed atom i into the electron density ρ and $\phi_{ij}(R_{ij})$ is the core-core repulsion between atoms i and j separated within the distance of R_{ij} [27].

The most conventional potential function for SiC has been developed by Tersoff. This force-field is able to model the interactions between silicon and carbon atoms in the structure. The value of energy between atoms i and j in this potential is calculated through:

$$V_{ij} = f_c(r_{ij})[f_R(r_{ij}) + b_{ij}f_A(r_{ij})] \tag{2}$$

where f_c, f_R, f_A, r_{ij} and b_{ij} represent the cutoff function, attraction force, repulsion force, distance between atoms i and j and local atomic environment function [28,29].

In 2007, Vashishta et al. developed a potential function to model both the crystalline and amorphous behavior of silicon carbide. Regarding the capabilities of this potential function to model different structures, investigating its behavior in modeling the shock wave sintering process is a matter of interest for the