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2014

Tang, C., Li, B., & Wong, C. H. (2014). Selective Laser Melting of Metal Powders Studied by Molecular Dynamics Simulation. Proceedings of the 1st International Conference on Progress in Additive Manufacturing (Pro-AM 2014), 291-296.

<https://hdl.handle.net/10356/84265>

https://doi.org/10.3850/978-981-09-0446-3_014

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SELECTIVE LASER MELTING OF METAL POWDERS STUDIED BY MOLECULAR DYNAMICS SIMULATION

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ABSTRACT

Selective laser melting can be used to build up 3D metal parts by melting metallic powders together. In this paper, we performed molecular dynamics simulation to investigate the selective laser heating process of Cu powders. Cu atoms were heated up by a mobile laser beam and subsequently cooled down by a Ni-base plate underneath them. Radial distribution function analysis revealed that Cu atoms are melted by the laser irradiation. Additionally, our results showed that Cu atoms around the laser beam are fused together.

INTRODUCTION

Over the past decades, selective laser melting (SLM) techniques have been used to create metallic components with complicated shapes [1]. To perform 3D printing, a SLM machine firstly places a layer of powders on the substrate. Then a focused high-power laser pulse is applied on the layer, which melts the powders according to a 3D CAD model. After the laser beam is removed, the melt solidifies quickly and forms a solid part, since the heat flux can be easily extracted by the substrate. By repeating these three procedures, a component with designed structure can be fabricated. For instance, Simon Pauly et al. [2] have fabricated a glassy metallic scaffold by using SLM.

Recent studies have shown the potential of molecular dynamics (MD) to investigate the behaviors of nano-materials such as carbon nanotubes [3-11] and metallic glasses [12-16]. They have also been adopted in the studies of nano-friction [17] and molecularly thin nanofilms [18-20]. Additionally, there were also reports on how MD have been employed in the studies of laser melting [21,22] such as the resultant depletion of lubricants due to laser heating [23-26]. With the strong evidence of suitability of MD to investigate nano-systems, therefore in this work, we employed MD to simulate the SLM process of Cu powders. The model consists of a Ni-base plate and some Cu powders placed on the substrate. After the model was equilibrated, a mobile laser beam was applied on the Cu powders. The heat source was then removed, and the system was further relaxed by the substrate. The evolution of Cu atoms during the SLM treatment has been extracted and studied in this work.

Figure 1 Schematic of the SLM model used in the MD simulations. (a) Top view of the equilibrated system; (b) cross-section view at the middle plane $y = 14.4$ nm. Cu and Ni atoms are colored pink and cyan, respectively. Each large pink sphere represents a Cu powder. The red region describes the initial position of the laser beam. The region enclosed by the dashed rectangle is shown in details in the inset.

SIMULATION MODEL AND METHODOLOGY

A system consisting of 179,600 Cu atoms and 163,020 Ni atoms was constructed to simulate the SLM process, as illustrated in Figure 1. The Ni-base plate with size of $43.32 \text{ nm} \times 28.88 \text{ nm} \times 1.48 \text{ nm}$ was used to cool down the Cu atoms. Fifty large spheres with the same radius of 2.16 nm were used to represent the Cu powders. The Cu powders, each containing 3,592 Cu atoms, were placed on the surface of the bottom layer. Figure 1(a) and (b) present the top view and cross-section view of the equilibrated system, respectively. We employed embedded-atom-model (EAM) potentials [27] to describe the interatomic force fields. Periodic boundary conditions (PBC) were imposed in x and y directions, while a shrink-wrapped boundary condition was applied in z direction. The timestep was set to 2 fs. The system was firstly equilibrated at a constant temperature of 300 K for 10 ps by using a canonical (NVT) ensemble. After the relaxation, the model was further equilibrated using microcanonical (NVE) ensemble with Langevin thermostat for another 5 ps. The relaxation process was conducted to ensure that the final simulated results are unbiased by the initial configuration.

A two-step heating/cooling process was implemented to simulate the SLM of metal powders. Firstly, the laser irradiation process was facilitated by adding non-translational kinetic energy (fix heating method) to Cu atoms. For the simulations, a laser beam with radius of 5 nm was initially placed at $(x, y) = (11, 14.44) \text{ nm}$, as shown in Figure 1(a). Subsequently, the heat source moved along the x direction with a velocity of 0.1 nm/ps . The laser heating duration is 200 ps with a power of 400 eV/ps. By using Langevin thermostat, the Ni-base plate was kept constant at 300 K to cool the melted powders caused by the high-power laser treatment. After the laser treating process, the laser power was removed from the system for it to cool down while the Ni-base substrate remained at 300 K. The duration of this cooling process is 100 ps. Both the heating and cooling process were modeled under NVE ensemble.

RESULTS AND DISCUSSION

Temperature profile

Local temperature evolutions of Cu atoms during the SLM process are analyzed, as shown in **Error! Reference source not found.** We compute the average temperatures of Cu atoms in three different

regions. A, B and C represent three cylindrical regions with the same radii of 2 nm. Their central axes are placed at $(x, y) = (11, 14.4)$ nm, $(x, y) = (21, 14.4)$ nm, and $(x, y) = (31, 14.4)$ nm, respectively. Their bottom and top are respectively located at $z = 1.48$ nm (this value corresponds to the top surface of the substrate layer) and $z = 5.78$ nm.

The figure clearly reveals the effects of laser pulse on local heating. As illustrated by the plot, atoms around the heat source are rapidly heated up to a high temperature (above 2000 K). As the laser beam moves far away from the locally heated region (or the laser beam is removed), local Cu atoms are cooled down at a relatively high cooling rate. Additionally, since the peak temperatures of those heated regions are much higher than the melting temperature of Cu ($T_m = 1358$ K), it is expected that Cu atoms around the laser beam would melt and subsequently be frozen during the SLM treatment.

Figure 2 Time dependence of temperature of Cu atoms in different regions during the SLM process.

Radial distribution functions

Radial distribution functions (RDFs) are commonly used to describe the correlation between atoms. Unlike crystals, whose RDFs typically show discrete features, liquids or amorphous materials could be characterized by relatively uniformly distributed RDFs [28]. To investigate the structural features of Cu atoms under laser irradiation, we plot the partial RDFs of Cu-Cu in region C at different moment, as shown in **Error! Reference source not found.**. The result at $t = 0$ ps indicates that the initial structure of the Cu atoms in region C is crystal-like. At $t = 200$ ps (when region C reaches the highest temperature), the partial RDF shows that Cu atoms in the region becomes liquid-like. Furthermore, as the region is quenched by the substrate ($t = 300$ ps), those melted Cu atoms are frozen and form an ordered structure.

Figure 3 Partial RDFs of Cu-Cu pairs in region C at different moments. The volume of region C is used as an approximate value to calculate the partial RDFs.

Structural evolution during SLM

Figure 4 depicts the top and cross-section views of the evolution of Cu powders during the SLM process from $t = 0$ ps to $t = 300$ ps. The coloring scheme adopted here is determined by the height of atoms. If Cu powders are melted, we can easily expect that the local average height of atoms would be lower, since the Cu atoms were fused together and fill the voids between the powders in the locally heated region. The simulation results indicate that Cu atoms around the laser beam are melted and subsequently cooled down by the substrate, as illustrated by Figure 4(a) and (b). For instance, Figure 4(b) shows the structure of the enclosed region depicted in Figure 4(a). Initially, the region maintains crystalline structure when the heat source is far away ($t = 0, 50$, and 100 ps). When the laser beam becomes close to the specific region ($t = 150$ and 200 ps), Cu atoms are melted and become amorphous. After the heat source is removed ($t = 300$ ps), the melted atoms are frozen quickly due to the substrate, forming an ordered configuration.

Figure 4 Structural evolutions of Cu atoms during the SLM process. (a) Top view and cross-section view of the system; (b) a detailed view of the enclosed region shown in the upper left diagram of (a). The color encodes the height of atoms during the SLM treatment.

CONCLUSION

The MD simulations studied in this work reveals the SLM process of Cu powders in details. The temperature analysis revealed that the focused high-power laser beam can quickly heat up the surrounding regions, leading to the local melting of Cu atoms. After the laser heating process is completed, locally melted atoms are frozen by the substrate Ni-base plate. Additionally, the RDF evolutions during the SLM process suggest that the structure of locally melted atoms become amorphous. Subsequently, those melted Cu atoms form crystalline arrays when they are cooled down by the substrate layer.

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