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Molecular dynamics simulation on the micro-structural evolution in heat-affected zone during the preparation of bulk metallic glasses with selective laser melting

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Abstract

The method of selective laser melting (SLM) is a new manufacturing technology which has been regarded as a potential candidate to prepare bulk metallic glasses (BMGs) without limit of critical dimensions. However, obstacles still remain since the crystallization is rather hard to be sustained in the heat affected zone (HAZ) during the preparation of BMGs, due to the existence of cyclic heating process. In order to find the possibility of inhibiting the crystallization behavior in the HAZ, the micro-structural evolution of $Ni_{75}Al_{25}$ metallic glass during the cyclic heating process at different temperature variation rates was studied with Molecular Dynamics (MD) simulation. The results reveal that at low temperature variation rates relatively, the crystallization begins during the heating or cooling process depends on the relaxation time between the glass transition temperature T_G and the maximum heating temperature T_{MAX}. The relaxation time also affects the transformation mode of crystal structure after the completion of crystallization behavior. When the temperature variation rate rises to 5×10^{13}K/s, the decline of nucleation occurred: during the heating process, the heating rate is so high that the nuclei at the low temperature could come into the embryo at the high temperature which lead to the fusion of crystal embryos. And the decline of nucleation provides a new possibility for the research on the inhibition of crystallization behavior in the HAZ during the preparation of BMGs with SLM.

Keywords: Selective laser melting; Molecular dynamics simulation; Bulk metallic glasses; Crystallization behavior; Decline of nucleation

1. Introduction

As a typical additive manufacturing technology, selective laser melting (SLM) has been regarded as a potential candidate to prepare bulk metallic glasses (BMGs) without limit of critical dimensions, due to its high heating and cooling rates in the small molten pool [1-5]. However, there are still some factors that hinder the application of this technique in the bulk amorphous preparation: during the multi-pass scanning of the laser, the deposited layer is subjected to the repeating heat of the molten pool, and the amorphous crystallization behavior is very easy to occur during the thermal cycling process, thus it is rather difficult to obtain complete amorphous structure in practical SLM process [6-10]. Since the thermal cycling process is unavoidable, the optimization of the forming process to suppress the crystallization behavior of the amorphous structure in the heat-affected zone (HAZ) during the thermal cycling process becomes the key to the breakthrough of this technology. However, the structure evolution during the crystallization process in the