Simulation and Experimental Verification of Grain Growth of

H13 Steel Electron Beam Surface Treatment

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Key words: electron beam,Monte Carlo method, grain growth, simulation,molten pool Abstract

Based on the actual electron beam scanning process of the surface of H13 steel specimen, a two-dimensional model of grain growth is established coupling Monte Carlo method. The crystallization of the molten pool is simulated after electron beam scanning of H13 steel, effects of scanning current and rate on the size of the molten pool are discussed. Results show that the bottom layer of the molten pool, and the upside is course equiaxed grains. The increase of the scanning current promotes the grain size and the increase of the scanning speed reduces the grain size. The grain size and growth direction of the gold phase are basically the same with the simulation results. Through the study of the grain growth of the molten pool on the surface of H13 steel scanned with electron beam, better process parameters and material properties can be obtained.

Introduction

Electron beam surface treatment technology is such a technology that makes a large amount of energy deposited at the thin layer of the material surface in a very short time, leading to physical and chemical changes of the material, the purpose of modification is thus realized[1]. In the melting process of the material surface, the size and microstructure of the grain will affect the performance of the material, therefore, research on the change of the microstructure during the solidification process of electron beam scanning has a significant meaning[2]. Based on Monte Carlo method (MC method), a two-dimensional model of grain growth is established, effects of process parameters such as scanning current and scanning speed on the molten pool grain are discussed, concurrently, experimental verification is carried out.

Establishment of grain growth model in electron beam scanning molten pool

Electron beam scanning process. Electron beam linear scanning process is shown in Fig.1. The electron beam current flow is perpendicularly shooting to the X-Y plane of the sample with a heat flow density q, and the sample moves down the negative direction of the Y axis with a velocity v, the driving signal is built by programming and continuous refresh rate is put to the X and Y pairs of winding, the magnetic field generated in the deflection yoke makes the electron beam moves regularly according to the set mode and trajectory in the X-Y plane.

Simulation area selection. Principles must be obeyed when selecting the grain

growth area in the molten pool are as follows[3]: the selected area must include all the characteristics of the molten pool after electron beam scanning process; to reduce the amount of computer calculation, the selected area should not be too large, the simulation area selected is shown in Fig.2. In the process of electron beam scanning, the simulation area starts from the center of the y direction and extends in the x, z direction by 1 mm.



Fig. 1 Schematic diagram of electron beam scanning

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Simulation area grain orientation initialization and discretization. The MC model divides the grid using the square spatial lattice[4]. After the discretization of the simulation area, a grain orientation number between 1 and Q is assigned randomly to each grid point. In the simulation process, the orientation of the microcell is initialized and the grain orientation number takes 28 [5].

Grid selection and reorientation. According to the difference of temperature, the simulation region is divided into three parts: solid state, liquid state and growth state. When simulating the growth, the order of grid selection is the same with that of solidification, that is, the grain grows from the bottom of the molten pool to the free surface. A random method is adopted when selecting the grid, the selected reorientation number is calculated according to the following formula[6]:

$$\begin{cases} p = 1 & (\Delta E \le 0) \\ p = \exp(-\Delta E/RT) & (\Delta E > 0) . \end{cases}$$
(1)

In the formula: ΔE is the difference of interaction energy before and after the orientation of the adjacent grid and grain changes (J), R is the Boltzmann constant (W/(m².k⁴)), usually taken as 5.67×10-8, P is the reorientation probability, T is the temperature of the liquid metal (K). The reorientation probability is determined by the grain boundary energy change before and after the reorientation obtained by the Hami operator, the change of the interaction energy is calculated by the following formula:

$$\nabla E = J \sum_{i=1}^{8} (\delta_{s_i s_0} - \delta_{s_i s_n}).$$
⁽²⁾

In the formula: J is the interaction energy of adjacent lattice points, S_0 is the original grain orientation number of the selected grid, S_i is the crystal value of the eight lattice points around the selected grid, S_n is the new crystal orientation value after the crystal orientation changes randomly, the reorientation probability can be obtained from (1) and (2).

Simulation results analysis and experimental verification

Simulation results analysis. In order to verify the reliability of the simulation MC model, constant temperature simulation is processed at first, the length of the unit is 100, the number of unit cells is 100×100 , the simulation time steps are 200, and the



simulation temperature is 500 K[3]. Changes of crystal size and quantity varying with the simulation time steps are shown in Fig.3.



Fig. 3 grain size distribution of different MCS

Experiment and results analysis. In this study, the experimental material is H13 die steel, its chemical composition is shown in Table 1.

Table 1 Chemical composition of H13 steel (wt%)								
С	Si	Mn	Cr	Мо	V	S	Р	Fe
0.32-0.45	0.82-1.2	0.22-0.5	4.75-5.5	1.12-1.75	0.8-1.2	< 0.03	< 0.03	Bal.

When the surface of H13 steel specimen is scanned with electron beam, the electron beam process parameters are as follows: the acceleration voltage is 60kV, the



Fig. 4 the morphology of grain growth of H13 steel weld pool by scanning electron beam surface treatment (a) test results; (b) simulation results

acceleration current 25mA, the scanning speed is 30mm/s, the beam spot diameter is 3mm, the scanning frequency is 100Hz, all of the scanning time is set 20s. The metallographic structure is observed by scanning electron microscopy (SEM), besides, the metallographic analysis is carried out. Based on constant temperature simulation, the temperature field data of H13 steel surface scanned by electron beam are extracted by software[7], the microstructure of the molten pool is simulated and the crystal state is shown in Fig.4 (b). It can be seen from Fig.4 (a) that after electron beam scanning process, there are fine equiaxed grains distributed at the bottom of the molten pool, which gradually transform into columnar crystal in the mid, and there are mainly coarse equiaxed grains in the upside. The bottom of the molten pool is close to the substrate, the temperature gradient is large and the cooling rate is fast, so the crystal is



small, however, the cooling rate in the middle of the molten pool is relatively slow, so the crystal is mainly columnar. The crystal orientation distribution of the experiment is basically consistent with the simulation results.

Effects of Electron Beam Scanning Parameters on Grain Growth

Effects of Scanning Current on Grain Growth. The scanning speed v is 20 mm/s, the beam spot diameter d is 3 mm, the acceleration voltage U is 60 kV, the scanning current I is respectively 15 mA, 20 mA, 25 mA, results are shown as follows:



Fig. 5 Effect of scanning current on average grain size Fig. 6 Effect of scanning current on grain

when the beam spot diameter and the acceleration voltage are constant, as shown in Fig.5, the average grain size increases as the current increases, because the increase of the scanning current leads to the increase of the temperature of the sample surface, the heat flux increases with the increase of the current, therefore, the maximum temperature of the electron beam scanning area rises, the heat energy of the transition increases, and the amount of heat from the scanning area spreading around rises, causing the reduction of cooling rate, then the grain growth time increases, the final grain is thus coarser. Fig.6 shows the microstructure of H13 steel under different scanning currents, the average grain size increases with the increase of scanning current, which is consistent with the simulation results.

Effects of Scanning Speed on Grain Growth. The acceleration current I is 30 mA, the spot diameter d is 3 mm, the acceleration voltage U is 60 kV, and the scanning speed v is respectively 15 mm/s, 20 mm/s, 25mm/s, results are shown as follows:



When the beam spot diameter and the acceleration voltage are constant, as shown in Fig.7, the average grain size increases as the scanning speed reduces. When



the scanning speed is small, the function time of the electron beam on the specimen surface becomes longer, the solidification time of the molten pool becomes longer, the cooling rate slows down, and the average grain size becomes larger. In the case of high scanning speed, the function time of the electron beam on the surface of the specimen becomes smaller, the solidification time of the molten pool is relatively short, the cooling rate increases and the average grain size becomes smaller. Fig.8 shows the microstructure of H13 steel under different scanning speed, the average grain size decreases with the increase of scanning speed, which is consistent with the simulation results.

Summary

(1) Monte Carlo model is adopted to simulate the constant temperature of the molten pool, the grain size distribution under different MC simulation time are obtained, the feasibility of the model is thus verified.

(2) By observing the microstructures of metallographic samples of H13 steel after surface treatment with scanning electron beam, we found that there are mainly fine equiaxed grains at the bottom layer of the molten pool, which transform into columnar crystals in the middle part of the molten pool, and there are mainly coarse equiaxed grains in the upside, the test results and simulation results coincide with each other.

(3) When the other process parameters are fixed, the variation trend of the average grain growth size is the same with that of the scanning current, the variation trend of the average grain growth size is opposite to that of the scanning speed, which are consistent with the experimental results.

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