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Effect of rare earth on B-Al permeating and computer kinetic simulation of permeation layer forming①

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Abstract: It was found that rare earth influenced per process of permeation layer forming, and that the tooth of layer was thinner, thicker, straighter and longer by observing permeation layers at different holding times. It was so image, lifelike and audio-visual by computer kinetic simulation that the layer forming could be continuously observed. Because it conforms to reality, the computer kinetic simulation can forecast the layer thickness and it will offer a reasonable permeating technology.

Key words: rare earth; B-Al; permeability; computer simulation **Document code: A**

1 INTRODUCTION

The study of effect of rare earth on microstructure, property and growth kinetic of the permeation layer (hereafter simplified as layer) has been reported in many papers[1~6] and there was a good effect in production use[7,8]. Rare earth-B-Al and B-Al alloys were compared, and layer forming was observed and effect of rare earth on microstructure and forming of layer were analyzed based on mature prescription[9] in this work. The change law of layer forming was shown imaginatively, lifelikely and audio-visually by computer kinetic simulation, so the layer thickness and reasonable permeating technology would be forecast and controlled.

2 EXPERIMENTAL METHODS

2.1 Specimen preparation

The dimensions of commercial iron specimens were d15 mm × 5 mm, and the surface finish was 1.6 μm. The specimens were heated for 0.5, 1, 2, 3 or 4 h at 920 ℃ with pasty and method shown in Ref. [9]. The accuracy of furnace temperature was ±5 ℃.

2.2 Layer thickness measurement

The metallograghic specimens were made after specimens were dissected along layer forming direction. The peaks of layer teeth of five representative visual fields were measured. The layer thickness was calculated by

$$y = \sqrt{y_1^2 + y_2^2 + y_4^2 + y_4^2 + y_5^2} \quad (1)$$

where y is layer thickness, and y_i are peak lengths of layer teeth. Deviation of y_i is 6 μm at 400 amplification visual field.

3 EXPERIMENTAL RESULTS

3.1 Effect of rare earth on thickness and microstructure

Table 1 shows the layer thickness and Fig. 1 shows the layer microstructures of B-Al and rare earth-B-Al at different holding times.

Table 1 Permeation layer thickness of B-Al and rare earth-B-Al (μm)

Permeation layer	Thickness				
	0.5 h	1 h	2 h	3 h	4 h
RE-B-Al	18	34	58	82	97
B-Al	12	17	37	58	76

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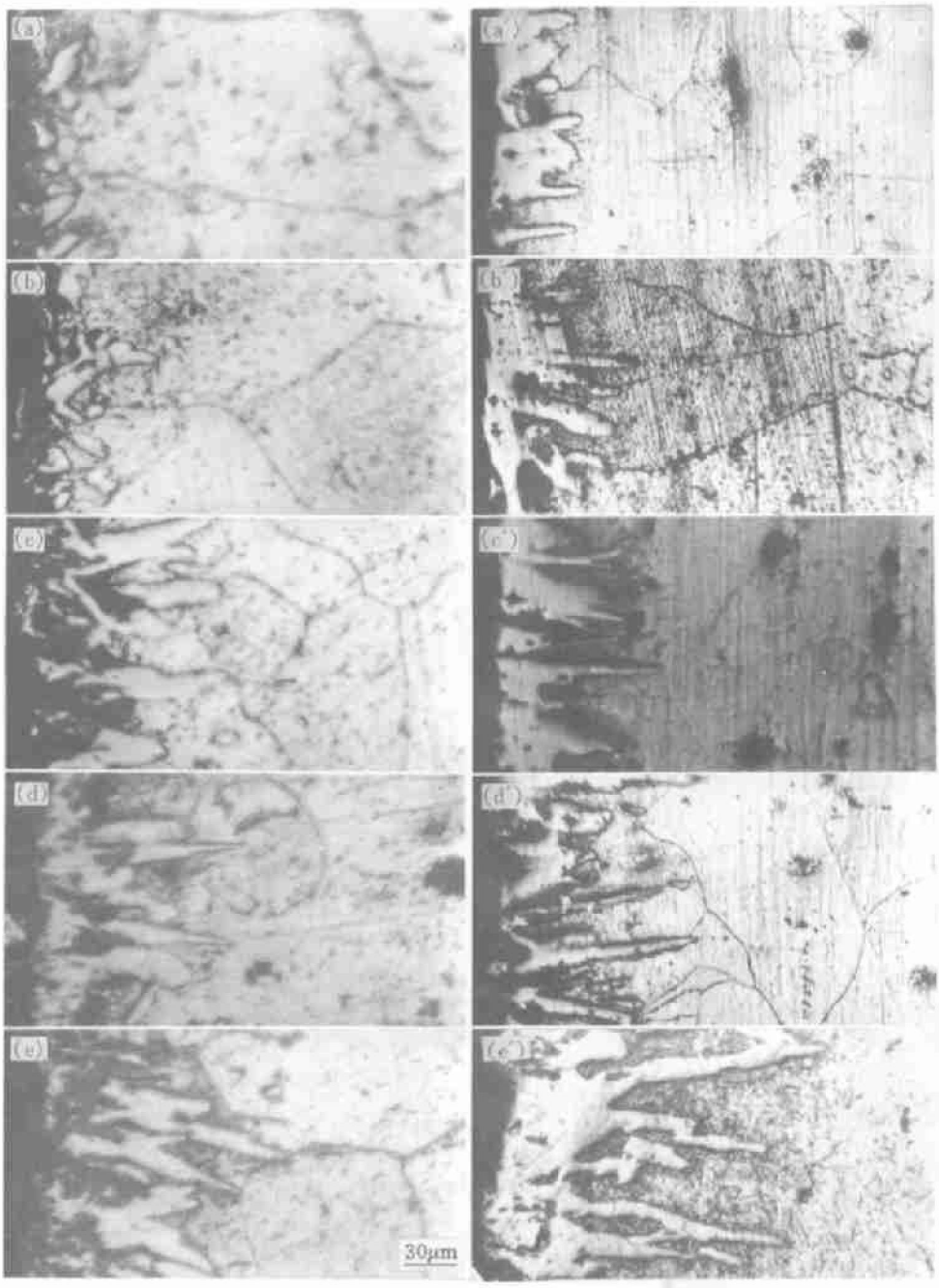


Fig. 1 Microstructures of permeation layer after holding at 920 ℃ for different times
B-Al: (a)—0.5 h; (b)—1 h; (c)—2 h; (d)—3 h; (e)—4 h
RE-B-Al: (a′)—0.5 h; (b′)—1 h; (c′)—2 h; (d′)—3 h; (e′)—4 h

As shown in Fig. 1, the layer of B-Al is thin, and the shape of tooth is loose, discontinuous and irregular. The difference of teeth peak heights is big and there are many independent

teeth that appear randomly and some of them are fork and oblique teeth. In opposition to B-Al, the layer thickness of RE-B-Al is increased obviously. The shape of tooth is continuous, regular, thin, fine and sharp, and the tooth roots of them are melt-grown.

Analysis shows that the thickness increasing and microstructure changing of layer are closely related to physico-chemical characteristics of rare earth in pasty. First, according to the rules of solid solubility and grain boundary, the rare earth atoms inevitably segregate at grain boundaries and micro-inhomogeneities (vacancy, dislocation) because the atom radius of rare earth is bigger than that of iron. Because of rare earth atoms enriching at grain boundaries, the lattice of iron atom around rare earth is enormously distorted so that [B] atoms are easily absorbed and solidified on the surface of specimens and first segregate in distortion areas. High concentration of [B] atoms at distorted areas pushes forward nucleation of boride and forms a lot of Fe_2B on specimen surface in the initial permeating stage. Second, as rare earth is a surface-active element, it is first absorbed on the surface of metal and the system energy is reduced during permeating. The rare earth atoms which have big absorption power around other atoms are easily absorbed on micro-inhomogeneities of specimen surface and form active centers. When the density of rare earth is suitable, the atoms absorbed by active centers covering specimen surface form active bodies around rare earth atoms again. [B] atoms which reach definite density diffuse into iron and then active centers absorb other [B] atoms so that a new system balance is established once more. As the above process, [B] atoms continuously diffuse into iron. All layers in all teeth become continuous, regular, thin, fine and tidy, and thickness of layer obviously becomes larger after the rare earth is added to pasty.

3.2 Establishment of growth pattern

Ref. [10] points out that [B] atoms powerfully segregate to defects of crystal and special grain boundaries. The test results[11] and analysis show that borides first nucleate at defects or boundaries of crystal on specimen surface in initial stage. If once composition and energy can be satisfied, borides would nucleate in grains. At this moment boride nuclei in grain boundary have become rather big. The first formed small nuclei which grow up in the preferred orientation are gobbled up by latter formed nuclei. Since they grows randomly, a portion of nuclei grow up horizontally at a large rate, collide with each other and then stop growth. The rest of them grow up to inner and simultaneously expand along the horizontal direction and the layer becomes teeth which contain a little other compounds forming during layer growth.

According to the above analysis, nucleation and growth of borides can be divided into two stages in this test if the effect of few complicated compounds is not considered. At the first stage, borides nucleate and grow up on the surface randomly, then at the second stage, boride teeth form and grow up by [B] atoms further extending. Rare earth affects both stages, first, the rare earth atoms increase the rate of nucleation and growth rate of nuclei, then since there is a large distortion around the rare earth atoms, [B] atom extending routes are formed , which improves extending of [B] atom according to characteristics of surface active theory.

4 COMPUTER SIMULATION

4.1 Original microstructure simulation

Computer with UGA indicator of 640×480 resolution draws original microstructure on two dimensional triangle lattice. Because it is displayed actively by multi-page, the picture is clear, image , lifelike and nearly looks real on a rectangle window whose length is diameter of field vision and width is measurement of lattice. As shown in Fig. 2, each one in the lattices is a small hexagon, so every lattice represents certain area. If the width of lattice is a unit length, every lattice represents certain volume again. Line segments 1～6 of Fig. 2 are boundaries of grain. Vector $\boldsymbol{n}$ is refinements of grain cell, vectors $\boldsymbol{m}_1 \sim \boldsymbol{m}_6$ are refinements of adjacent grain cells. If $\boldsymbol{n}$ equals $\boldsymbol{m}_1$, boundary 1 doesn't exist. The other boundaries are set in similar way by analogy.

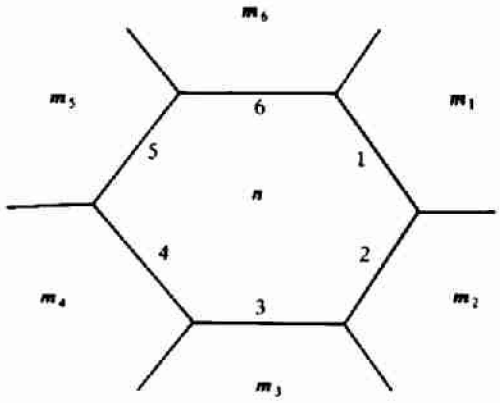


Fig. 2 Original composition simulation mode

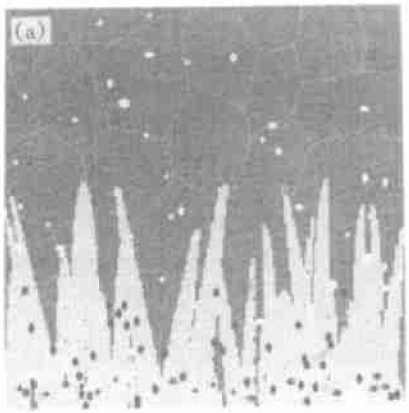
4.2 Mathematical simulation establishment of layer growth

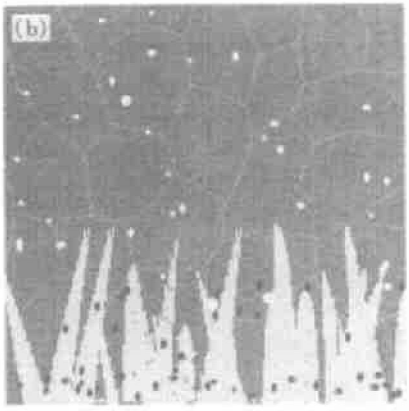
Mathematical simulation is an empirical formula or certain regular correspondent relation which represents parameters between test aim and characteristic. Whether the mathematical model is right or not directly affects the modeling results. Tables 1 and 2 respectively give the test data and approximate curve equations in this test condition.

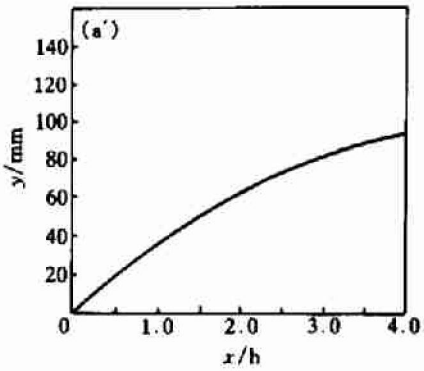
Table 2 Approximation curve equation

Permeation layer	Equation	Approximation degree
RE-B-Al	$y = -2.51x^2 + 33.96x + 1.96$	99.71%
B-Al	$y = 0.13x^2 + 12.54x - 0.13$	99.94%

y—permeation layer thickness, μm; x—permeation time, h







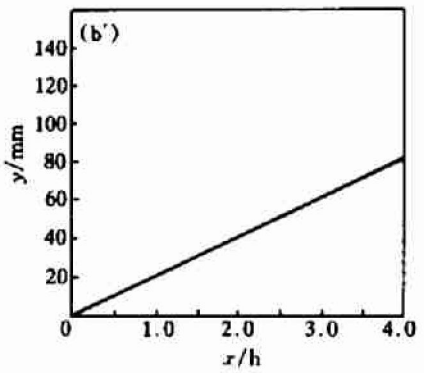


Fig. 3 Permeation layer forms of computer kinetic simulation and permeation layer approximation curves at different times
(a) and (a')—RE-B-Al; (b) and (b')—B-Al

These equations give the relation between time and layer thickness of permeating. Computer screen shows that the change of layer thickness curve with time and layer growth rate is synchronous. Layer thickness data can be read out by randomly selecting permeation time.

4.3 Simulation of layer growth process

According to the relation between the thickness of layer and the holding time, the growth of crystal nucleus can be controlled. This process can be simulated according to the following rules.

(1) Deciding if nucleation position selected randomly can nucleate: value 0, no nucleation; value not 0, nucleation on surface of specimen.

(2) Deciding orientation of adjacent particles: when orientation is vertical with the surface of layer, borides can grow continuously; when not vertical, most of borides stop growing because adjacent crystal nuclei contact each other.

(3) Eastablishing relation between layer growth rate v and holding time, $v = dy/dx$ decreases with time extending and is a decreasing function of time.

(4) Near growth rule: both adjacent teeth of borides merge when they contact each other in growing.

(5) Field of vision: deciding growth field where is not out of boundary of field vision according to relation between the growth rate and holding time.

Fig.3 presents layer forms of computer kinetic simulation and layer approximation curves.

5 CONCLUSIONS

(1) Boride tooth of RE-B-Al was tidier and finer, and layer growth rate was faster than that of B-Al.

(2) Mathematical model established according to test data realized computer kinetic simulation of layer thickness.

(3) Because it conformed to reality, computer kinetic simulation could forecast and control the layer thickness by selecting technology parameters.

(4) Layer forming of computer kinetic simulation was image, lifelike and audio-visual.

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