

Calculation of Surface Mismatch between Zirconium Alloy Matrix and Its Oxide Film

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[Abstract] In this paper, the calculation of the misalignment of the zirconium alloys of the two groups of A and B in different textures is carried out. According to the mismatch principle of film growth, the nucleation planes of the surface of the A combination alloy are mainly (200), (020), (002) three crystal planes, and the crystal plane mismatches with the growth crystal planes $(\bar{1}04)$, $(\bar{1}05)$, $(\bar{1}06)$ exceeds 65% ; on the other hand, the nucleation planes on the B-composite alloy surface are mainly (011), (110), (101), $(10\bar{2})$, and $(\bar{1}03)$ crystal planes, which are only 40% or lower with the growth crystal plane mismatch.

[Keywords] Zirconium alloy; Oxide film; Texture; Surface misfit

1. Introduction

Zirconium alloy fuel cladding tubes inevitably undergo several deformations and annealing during processing. After deformation or annealing, the zirconium alloy will correspondingly produce a textured texture and an annealed texture, which will directly result in different crystal faces parallel to the zirconium alloy table. Many scholars have found that zirconium alloys that are relatively low temperature annealed at 470 degrees have better corrosion resistance.^[1] These important results provide a very important experimental basis for the subsequent work, but the specific mechanism of improving the corrosion resistance of zirconium alloy by lower temperature annealing still needs further study. Based on the scientific and engineering nature of this work, this work used two different annealing temperatures of zirconium alloy for 200 days of corrosion. The nucleation growth of the alloy texture and its oxide film was analyzed to discuss the effect of annealing at different temperatures on the corrosion resistance of the alloy.

2. Experiment and Method

Zr-Sn-Nb-Fe-Cu-O alloy was selected as the experimental alloy for this work. The cold rolled alloy sheet thickness was 0.6 mm, and then the alloy was cut into two parts and annealed using two temperatures. A portion was annealed at 570 °C for 5 hours and recorded as Group A; the other portion was annealed at 470 ° C for 5 hours and recorded as Group B. Bramfitt et al. optimized the single crystal mismatch formula to the matte mismatch formula, which essentially considers the average mismatch between the three crystal orientations of the two bonded crystal faces. The formula for the mismatch formula is as follows:

$$\delta_{(hkl)_n}^{(hkl)_s} = \sum_{i=1}^3 \frac{\left| d_{[uvw]_s^i} \cos \theta - d_{[uvw]_n^i} \right|}{\frac{d_{[uvw]_n^i}}{3}} \times 100$$

3. Results and Discussion

In this work, the A combination alloy and the B combination alloy only had different annealing temperatures, but the A combination alloy had a corrosion transition after 100 days, and the B combination alloy did not undergo a corrosion transition for 200 days after the end of the corrosion test. It shows that the corrosion resistance of B combination alloy is better than that of A combination alloy. The surface of the A combination alloy is parallel to the (0002) crystal plane, and this result can be directly obtained from the orientation of the positive electrode of the (0002) crystal plane. The close-packed hexagonal c-axis of the B group alloy is inclined from the ND direction of the sample to the TD direction. The parallel crystal planes of the B combination alloy and the sample surface were calculated by using a unit cell of a hexagonal hexagonal shape ($\bar{1}\bar{1}02$), ($\bar{1}\bar{1}03$), and ($\bar{1}\bar{1}04$). Therefore, the nucleation of the oxide film will mainly occur from these crystal faces.

We have selected a large number of low-index crystal faces to match the (0002), ($\bar{1}\bar{1}02$), ($\bar{1}\bar{1}03$), and ($\bar{1}\bar{1}04$) mismatches of zirconium alloy unit cells. Then compare the results. From the results, it was found that the crystal faces having different misalignments with the monoclinic zirconia were different on the crystal faces of the substrate. Obviously, on the (0002) crystal plane of the substrate, the (200), (020) and (002) crystal faces of the monoclinic zirconia have the smallest mismatch.

For the ($\bar{1}\bar{1}02$) crystal plane of the matrix, the (011), (110) and (101) crystal faces of the monoclinic zirconia have the least mismatch with the surface;

For the ($\bar{1}\bar{1}03$) crystal plane of the substrate, the ($\bar{1}02$), (011) and (101) crystal faces of the monoclinic zirconia have the least mismatch with the surface;

For the ($\bar{1}\bar{1}04$) crystal plane of the substrate, ($\bar{1}02$) and ($\bar{1}03$) of the monoclinic zirconia have the smallest mismatch.

In order to maintain stability, the nucleation will select crystal planes with low mismatch.

The texture of the oxide film of the zirconium alloy corrosion sample after 70 days of autoclave corrosion is similar, especially the ($\bar{1}04$), ($\bar{1}05$), and ($\bar{1}06$) of the A group sample and the B group sample oxide film are parallel to the normal direction of the sample. The only difference is that the texture strength of the B group samples is slightly higher than the A group samples. If on the substrate, the (0002) crystal plane

of the zirconium unit cell is parallel to the surface of the sample, the mismatch of the surface between the nucleation crystal plane and the growth crystal plane exceeds 60%, indicating that the degree of distortion is high.

when the $(1\bar{1}02)$ or $(1\bar{1}03)$ crystal plane of the zirconium unit cell is parallel to the surface of the sample, the surface mismatch between the nucleation crystal plane and the growth crystal plane is reduced to about 40%;

And when the $(1\bar{1}04)$ crystal plane is parallel to the surface of the sample, the misalignment between the nucleation plane and the growth plane is further reduced.

This means that the degree of distortion between the nucleation plane and the growth plane is correspondingly reduced. From this result, it can be seen that if the c-axis of the zirconium unit cell is deflected to a certain angle in the TD direction of the sample along the ND direction of the sample, the degree of distortion and the number of defects in the growth process of the zirconia grain can be greatly reduced.

4. Conclusion

The (0002) crystal plane of the group Z zirconium alloy zirconium unit cell is mostly parallel to the sample surface, and the (0002) crystal plane of the group Z zirconium alloy zirconium unit cell is inclined by 25 to 40° in the TD direction along the ND direction of the sample. , converted to the sample $(1\bar{1}02)$, $(1\bar{1}03)$, $(1\bar{1}04)$ high probability parallel sample surface. The mismatch between the nucleation surface of the alloy oxide film of A and the growth crystal plane is larger than 65%; The mismatch between the nucleation surface of the B-alloy oxide film and the growth crystal face is small, about 40% or even lower.

References

- [1] Liangyu Chen, Jiuxiao Li, Yao Zhang, Lai-Chang Zhang, Weijie Lu, Lefu Zhang, Liqiang Wang, Di Zhang. Effects of alloyed Si on the autoclave corrosion performance and periodic corrosion kinetics in Zr-Sn-Nb-Fe-O alloys[J]. Corrosion Science, 2015, 100(2):651-662.