Sr Study on the Metamorphic Mechanism of Eutectic Silicon in Hypereutectic Al-Si Alloys

Mengjun Zhang[1,2], Zhiyong You[1,2,*], Yunguan Zhang[1,2], Libo Wang[1,2]
1. School of Materials Science and Engineering, Taiyuan University of Technology, Taiyuan 030024, China
2. Key Laboratory of Interface Science and Engineering in Advanced Materials Ministry of Education, Taiyuan University of Technology, Taiyuan 030024, China
*E-mail:13603511486@163.com

Abstract: The addition of a Sr modifier during the forming process of a hypereutectic Al-Si alloy results in the transformation of the acicular eutectic silicon within the alloy structure into rod or particle form. This process leads to an improvement in the comprehensive mechanical properties of the alloy. However, there is a lack of research on the mechanism of eutectic silicon metamorphism, especially on the interaction between the modifier and silicon phase. In this paper, the structural stability of Si(100) clean surface and adsorption model surface is studied by using the first-principle calculation method based on density functional theory. The results show that Sr is easily adsorbed on the surface of silicon phase and tends to fall at the Vacancy site. Then, Al-15%Si alloys with different Sr content are prepared by metal mold casting. By observing the SEM scans of the microstructure of alloy samples, it is found that Sr atoms are completely adsorbed and enriched on the surface of eutectic silicon.

Keywords: Hypereutectic Al-Si alloy; microstructure; first-principle; surface property

1 Introduction

Hypereutectic Al-Si alloys have been widely used in the manufacture of engine components such as cylinders or pistons because of high specific strength, low coefficient of thermal expansion and wear resistance[1]. However, the microstructure of the hypereutectic Al-Si alloy comprises long acicular eutectic silicon which can result in the matrix being cut or cause stress concentration at its angular tip. Modification treatment is an effective way to modify the silicon phase morphology and improve the mechanical properties of hypereutectic Al-Si alloys. As a traditional eutectic silicon modifier, Sr can not only modify the morphology of eutectic silicon, but also act as a green and environmentally friendly modifier. Furthermore, it has long-term effectiveness. Yan et al[2] explored the nucleation and growth mechanism of silicon phase through morphology analysis and non-isothermal analysis kinetics, and the results showed that Sr modified eutectic silicon mainly in three aspects: (1) toxic nucleation sites; (2) the interface energy between Si phase and liquid is reduced; (3) improve the activation energy of solid-liquid interface diffusion.

2 Experimental procedure

In this study, the CASTEP calculation program is employed to perform first-principle calculations. The exchange correlation energy parameter selected in the geometric optimization process is the PW91 model. The plane wave energy of 300 eV and the Monkhorst-Pack of 6×6×6 are selected as the truncation energy and k-point grid of the volume phase calculation, respectively.

Then ZL109 material was selected as the master alloy, and Al-15%Si alloys were prepared by adding Al-30%Si. Sr modifier is added in the form of Al-10Sr alloy. The Al-15%Si alloys containing 0.03%, 0.06% and 0.09% (wt.%) Sr were prepared by metal mold casting. The microstructure of the alloys were analyzed by SEM scanning.

3 Results and discussion

The Si(100) clean surface and the surface of the adsorption model corresponding to three different adsorption sites were constructed, as shown in Figure 1.

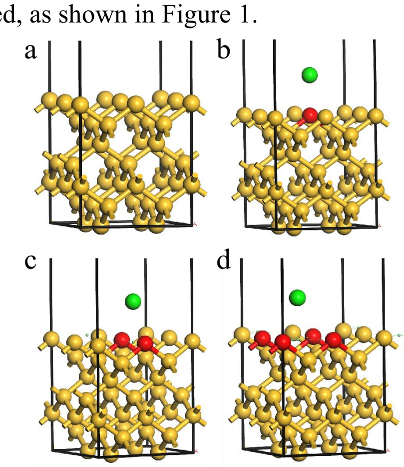

Fig. 1 Si(100) clean surface and adsorption surface model: (a) clean surface; (b) Top site; (c) Bridge site; (d) Vacancy site(The green atom is Sr atom and the rest are Si atoms)

The adsorption energy and surface energy of different surface models are calculated to determine the effect of Sr on the surface stability of silicon phase. The calculation formulas are shown in equation (1) and equation (2).

$$E_{ad} = E_{Sr/Si(1\,0\,0)} - E_{Sr} - E_{Si(1\,0\,0)} \qquad (1)$$

$$E_{surf} = \frac{E_{Sr/Si(1\,0\,0)} - E_{Sr} - N_{slab}E_{Si}}{2A} \quad (2)$$

E_{ad} is adsorption energy; $E_{Sr/Si(100)}$ is the total energy of adsorption model; E_{Sr} is the energy of a single Sr atom; $E_{Si(100)}$ is the total energy of clean surface; E_{surf} is the surface energy; N is the number of Si atoms; A is the surface area of the surface model.

The adsorption energy and surface energy of different surface models are shown in Table 1. As shown in Table 1, the adsorption energy and surface energy of the vacancy site adsorption surface model are both the smallest, which are -1.98 eV and 0.04 eV, indicating that Sr atoms are easily adsorbed on the surface of silicon phase and are more inclined to fall at the vacancy site of silicon phase.

Table 1. Calculation results of adsorption energy and surface energy of different surface models

Model	a	b	c	d
E_{ad}/eV	-	-0.76	-1.32	-1.98
E_{surf} /eV	0.06	0.06	0.05	0.04

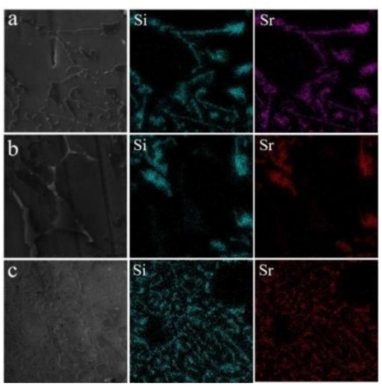

Fig.2 SEM scanning images of alloys after modification with different content of Sr: (a)0.03% (b)0.06% (c)0.09%

The SEM images of the three Sr modified alloy are shown in Figure 2. It can be seen that the positions and distributions of Si and Sr atoms in the alloy completely overlap, which indicates that after adding Sr atoms in the forming process of hypereutectic Al-Si alloy, all Sr atoms will be absorbed and enriched on the surface of silicon phase.

4 Conclusion

（1）Sr atoms easily adsorb on the surface of the silicon phase and tend to fall at the vacancy site of the silicon phase.

（2）The SEM images confirm the above view and show that Sr atoms are fully adsorbed and enriched on the surface of the silicon phase.

5 Acknowledgments

This work is supported by the 2021 Central Government Guide local science and technology development Fund (YDZJSX2021A008) and key Laboratory of Interface Science and Engineering in Advanced Materials Ministry of Education

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