STRUCTURAL TRANSFORMATION AND ITS REVERSIBILITY IN LIQUID Al-13%Si ALLOY AT HIGH TEMPERATURES①

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ABSTRACT Using high temperature X-ray diffraction analysis, the liquid structures of Al-13%Si alloy at 625~ 1 250 ℃ on heating and those at 675 ℃ after overheating of various temperatures were presented. It is shown that the atomic density and coordination number of the melt increased slightly at first, then decreased greatly at 775~ 875 ℃. The liquid structure of the melt at 675 ℃ and the morphology of the solidified alloy had no obvious change after overheating at various temperatures. These results indicate that structural transformation happens in liquid Al-13%Si and it is reversible.

Key words Al-13%Si alloy structural transformation X-ray diffraction analysis

1 INTRODUCTION

Having good mechanical properties and perfect foundry technological properties, the eutectic Al-Si alloys are often used for manufacturing thin-walled and complex-shaped parts which do not require high strength. The mechanical properties of the Al-Si alloys depend on the size and morphology of the Si phase in solid state. The process of producing metal parts often starts from liquid state, and there is hereditary effect of the liquid phase on the following solid phase[1]. Therefore it is important to study the structure and properties of liquid Al-Si alloys. There are some theoretical methods, such as molecular dynamics and Monte Carlo simulation calculation, and experimental methods including X-ray diffraction, electron diffraction and neutron diffraction[2]. The literatures about liquid structure of Al-Si alloys using X-ray diffraction are few, and sometimes contradict with each other[3-5].

This paper studied the liquid structure of Al-13%Si melt at 625~ 1 250 ℃ and at 675 ℃ after overheating at various temperatures, then studied the microstructures in solid state after solidification.

2 EXPERIMENTAL

Al-Si alloy samples were cast from Al ingot (99.999% in purity) and single crystal silicon (99.999% in purity) in SiC crucible. X-ray diffraction measurements were carried out in high purity helium atmosphere of 1.3×10^5 Pa. The specimen was placed in an alumina crucible of 30mm × 25mm × 8mm in size, using Ta sheet as heating elements. Surface of the specimen was fitted to a horizontal position using laser calibrator. Some other parameters of the diffraction experiment included: X-ray tube with MoK_α (λ= 0.0709 nm) and counter synchronized with each other (θ-θ), graphite mosaic monochromator

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crystal, voltage of X-ray tube 40 kV, current 30 mA, exposure time 30 s, measured angle from 0 to 90°. The temperatures of experiment are shown in Table 1.

Table 1 Temperature of X-ray diffraction

No.	1	2	3	4	5	6	7	8
Overheating temperature/ ℃	–	–	–	–	–	775	875	1 250
Temperature of diffraction/ ℃	625	675	775	875	1 250	675	675	675

The X-ray scattering intensity in experiment was measured in arbitrary units, and it was normalized into $S(Q)$, then converted to the pair correlation function $g(r)$ and radial distribution function $4\pi r^2\rho(r)$ with Fourier integral. Coordination number and atomic density of the liquid were calculated from the radial distribution function using the method described in Ref. [6]. The former is the integration of $4\pi r^2\rho(r)$ from the nearest zero left to the first peak.

3 RESULTS AND DISCUSSION

3.1 XRD analysis of structural transformation of Al-Si melt on heating

Fig. 1 shows the total structural factors $S(Q)$ of Al-13% Si in the range of 625~1 250 ℃; Q is a diffraction vector, equal to $4\pi\sin\theta/\lambda$. There are two peaks on curve, the first is higher and the second is lower. With increasing temperature, the heights of peaks decreased a little at first, then decreased drastically at 775 ℃, see Fig. 2.

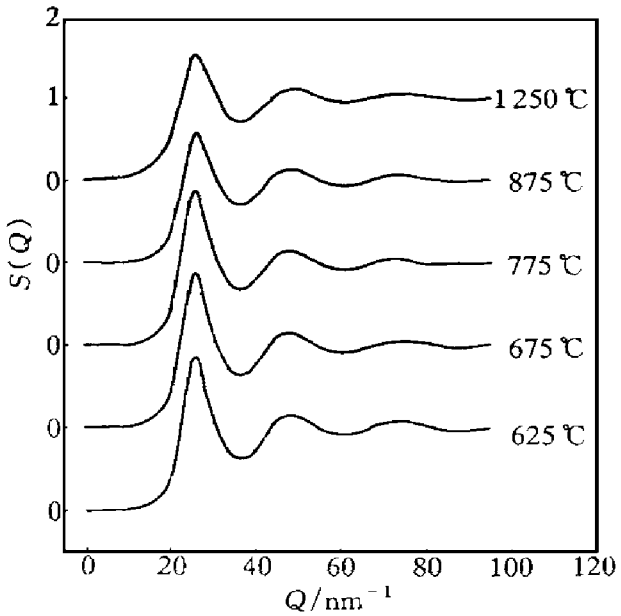

Fig. 1 Total structureal factors $S(Q)$ of Al-13% alloy at various temperatures

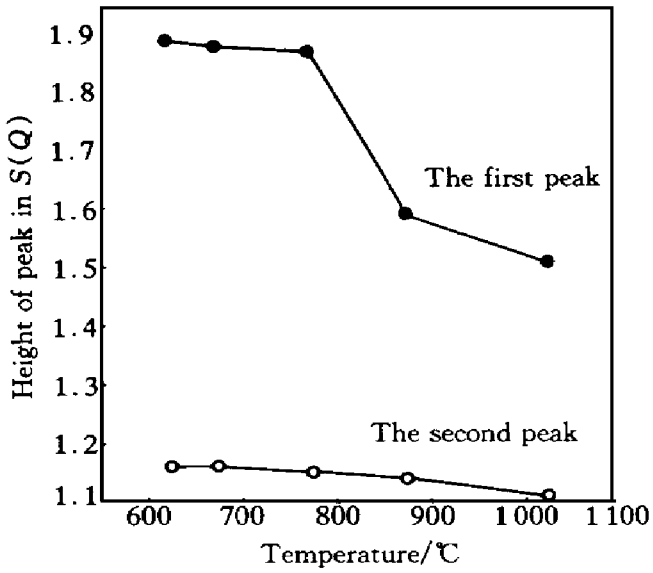

Fig. 2 Heights of peaks in $S(Q)$ at various temperatures

Fig. 3 depicts the pair correlation function $g(r)$ of the Al-13% alloy at various temperatures ranging from 625 ℃ to 1 250 ℃, the horizontal axis is the distance r of an atom from the referred atom, the vertical axis is the appearance possibility of the atom at r. The heights of the two peaks decrease nonlinearly and their

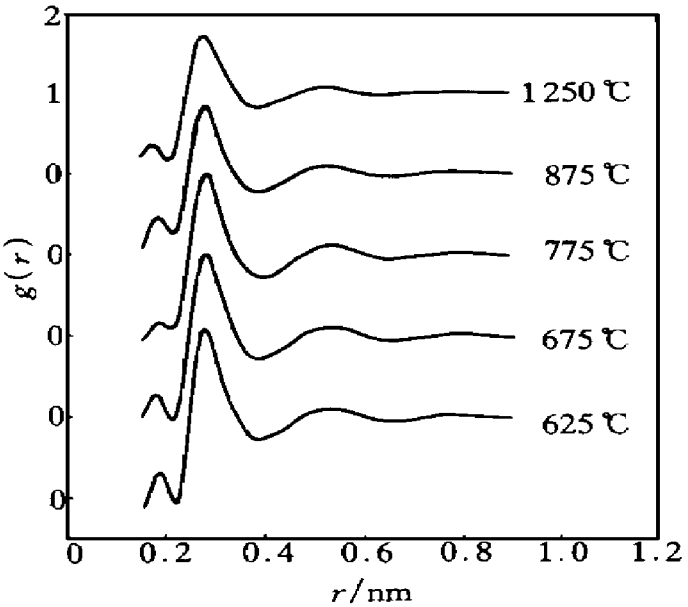

Fig. 3 Pair correlation functions $g(r)$ at various temperatures

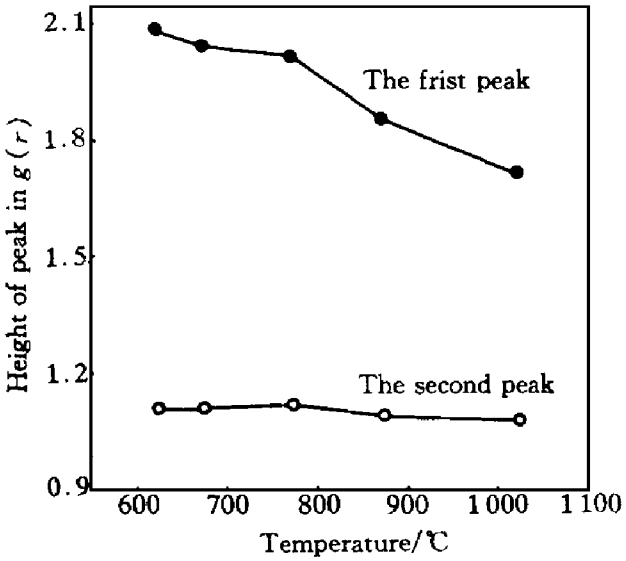

Fig. 4 Heights of peaks in $g(r)$ at various temperatures

positions do not change obviously with increasing temperature. Fig. 4 shows that a significant decrease of the height occurs at 775~ 875 ℃, like that in the case of $S(Q)$.

The total structural factors $S(Q)$ were Fourier-transformed to give the radial distribution functions $4\pi r^2\rho(r)$ (see Fig. 5). From Fig. 5, we can calculate the mean atomic density ρ_0 (the number of atoms per volume unit) and the coordination number n_c (number of nearest atoms around one atom), see Fig. 6. They decrease greatly at 775~ 875 ℃ with increasing temperature.

3.2 Reversibility of structural transformation on cooling

In order to know more about the structural transformation of the liquid Al-13% Si alloy, the structural parameters of the melt after holding for long times at 675 ℃ following overheating at various temperatures and the microstructures of the solidified alloy are shown in Table 2 and Fig. 7. The parameters of the melt do not change clearly although the difference between the overheating temperature is great and the following microstructures in solid state also do not change greatly.

3.3 Discussion

"The experiential electronic theory of solids and molecules" proposed by Prof. Yu Ruihuang

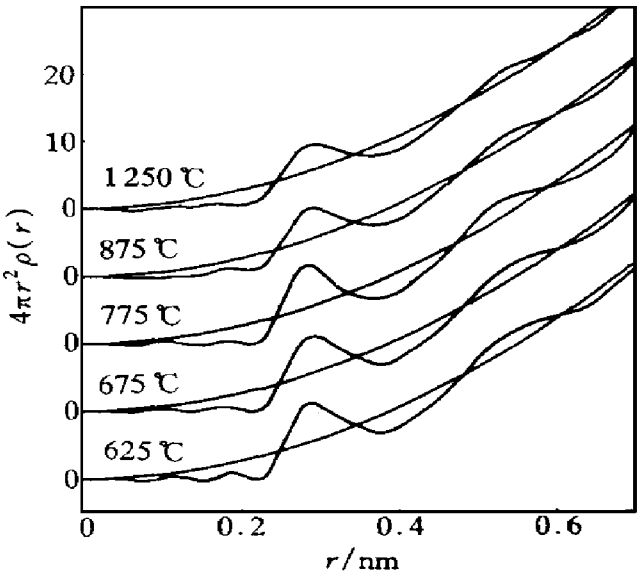

Fig. 5 Radial distribution function $4\pi r^2\rho(r)$ at various temperatures

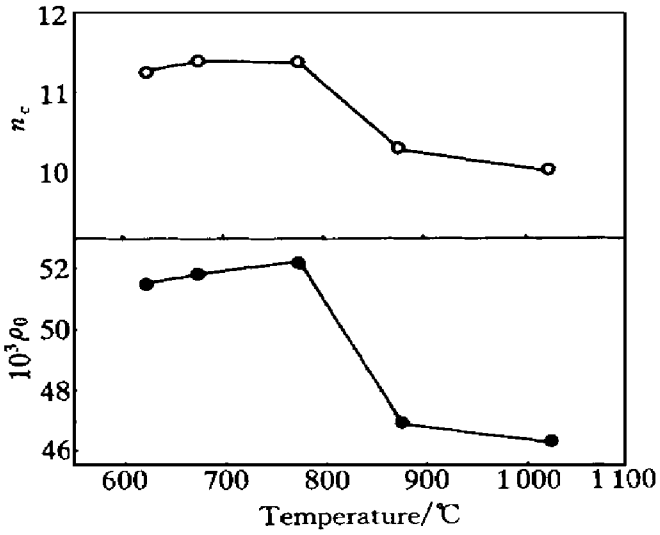

Fig. 6 Mean atomic density ρ_0 and coordination number n_c of alloy at various temperatures

Table 2 Structural parameters at 675 ℃ after overheating at different temperatures

Overheating temperature/ ℃	No overheating	775	875	975	1 275
Atomic density/A^{-3}	0.051 8	0.051 6	0.051 5	0.051 9	0.051 7
Coordination number	11.375	11.350	11.400	11.343	11.380

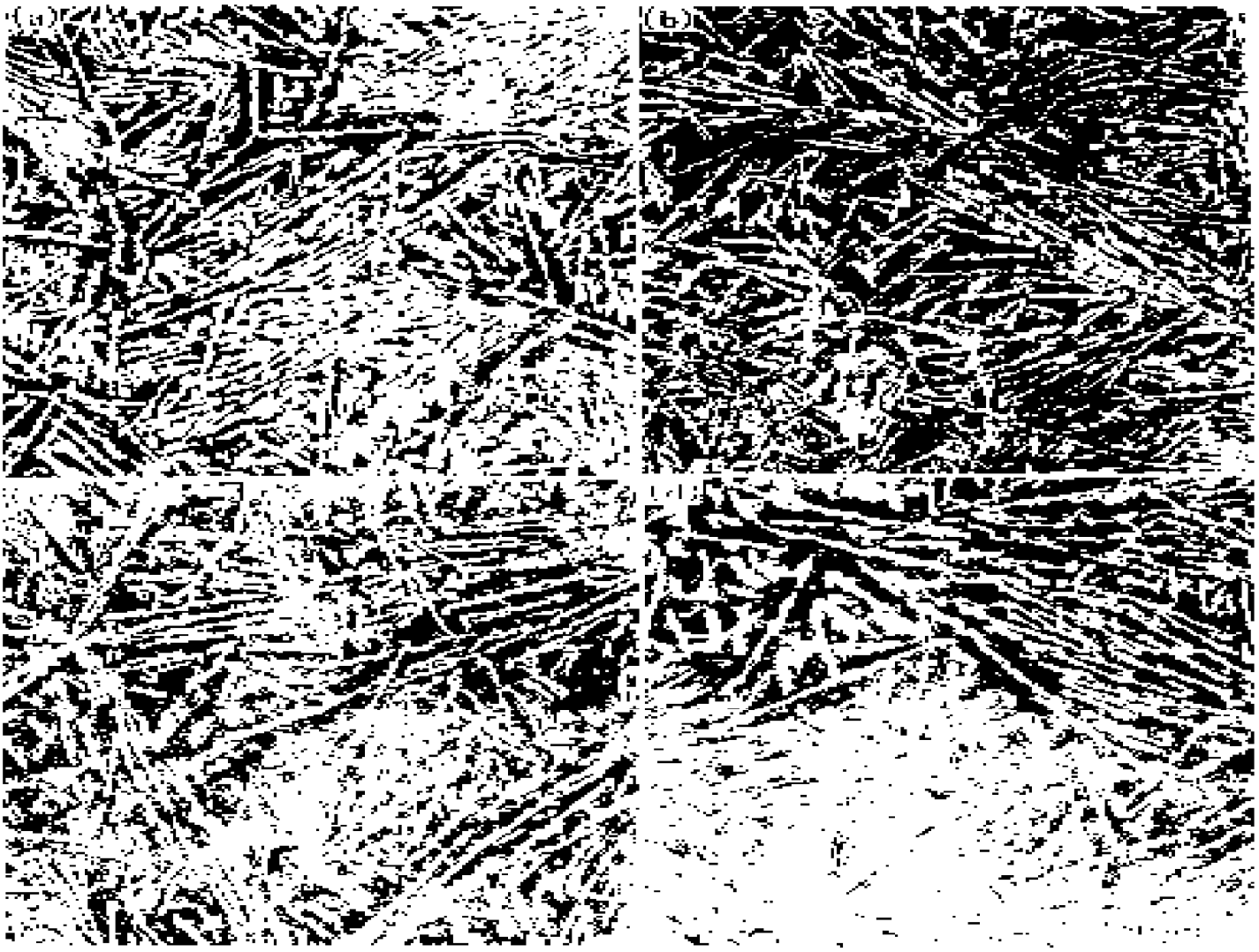

Fig. 7 Microstructures of Al-13% Si alloy solidified from the melt after holding for long time following overheating at various temperatures

(a) —No overheating; (b) —775 ℃; (c) —875 ℃; (d) —1 250 ℃

considers the state of atoms in molecules and solids depend on the bonding factor and size factor, which results in the bonding nets in molecules and solids. Yu thinks the melting process of the crystal is rather the break of the dominated bonds of the lattice in three-dimension periodic order than the separation of the atoms in crystal into single units. The position of the first peaks in $g(r)$ is ~ 0.280 nm, as shown in Fig. 3, close to the value in solid state (0.286 nm), which means survival of bonds in the liquid state. It has been demonstrated that there were Si-Si clusters in Al-Si melt by centrifugalization method[8]. It is known that the X-ray diffraction spectrum of Al-Si alloys in solid state has individual Al peaks and Si peaks, which become much lower when the alloys transform to liquid, and combine to a wider peak (i.e. the first peak in $S(Q)$ curve). This suggests that the first peak in $S(Q)$ reflects the information about the total nearest relation of Al-Al, Al-Si, and Si-Si, and that the number of the Al-Al, Al-Si and Si-Si bonds.

With increasing temperature, the heights of peaks decreased slightly at first, suggesting that the break of the bonds happened in the melt and that Si atoms diffused from Si-Si clusters into the Al bulk melt. During the diffusing process, some old Si-Si bonds had been destroyed while some new Al-Si bonds were produced. At 625~775 ℃, decrease of the peak heights in $S(Q)$ is not obvious, meaning the number of the

destroyed bonds is close to that of the produced bonds. At the same time, the coordination number of the melt increases slightly up to 11.30, see Fig. 5 and Fig. 6, while coordination numbers of pure liquid Al and Si are 11.5 and 4.8~5.8 separately[9]. From this fact, it can be deduced that the Si atoms occupy the positions of Al atoms in the bulk melt after leaving the Si-Si clusters.

When the temperature was high enough, the heights of first peaks in $S(Q)$ and $g(r)$ decreased greatly at 775~875 ℃, while the same changes of the atomic density and coordination number happened. This means that the dissolving process of the Si-Si clusters reaches the limit, and the structural change of the melt is dominated by the reducing of the old bonds with producing few new bonds.

After holding at 675 ℃ for certain long times under overheating at various temperatures, the structures of the melt is reproduced like that under no overheating. The microstructure in solid state at the same cooling rate remains unchanged. These illustrate that the dissolving of the Si-Si clusters in the Al-13%Si melt is in two directions, reversal, accompanied by the depositing process like that in the dissolving of the crystal in the solution. The bond in melt might be destroyed by the thermal oscillation of the atoms, while new bonds are produced when atoms contact each other. The number of the old destroyed bonds is higher than that of the newly produced bonds on heating, while the case is on the contrary on cooling.

4 CONCLUSIONS

(1) With increasing temperature, the atomic density and coordination number of Al-13% Si alloy increase slowly at first, then decrease greatly at 775 ℃. These suggest that the liquid structure has changed, which is caused by the dissolving of Si-Si clusters into the Al bulk melt.

(2) After holding at 675 ℃ for certain long time under overheating at various temperatures, the liquid structure of Al-13% Si melt is the same, and the microstructure of the solidified alloy is also the same. This shows that the structural transformation happening at high temperatures is reversal.

REFERENCES

1 Bian Xiufang, Liu Xiangfa, Wang Xian'e and Ma Jiaji. Acta Metall Sinica, (in Chinese), 1997, 33(6), 614.

2 Lu Kunquan. Physics, (in Chinese), 1994, 23(5): 264.

3 Ватолин Н А, Пастухов Э А, Серцягин В Н. Доклады АН СССР, 1975, (3): 641-643.

4 Пригунова А Г, Мазур В И, Таран Ю Н, Ростовская Л А, Персион Э В, Христенко Т М, Романова А В. Металлофизика, 1983, 5(1): 88-94.

5 Крушенко Г Г, Шаков В И, Никитин В И, Торшидова С И. Изв АН СССР Металл, 1977, (4): 204-207.

6 Ilinsky A G, Korobov V A and Slyusarenko S I. Met Phys Adv Tech, 1996, 15: 817-823.

7 Zhang Ruiling. The Experiential Electronic Theory of Solids and Molecules, (in Chinese). Changchun: Jilin Press of Science and Technology, 1993: 279.

8 Singh M and Kumar R. J Mater Sci, 1973, (8): 317.

9 Kita Y, Van Zytveld J B, Morita Z and Iida T. Phys: Condens Matter, 1994, (6): 811.

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