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Short communication

Quantification of precipitate fraction in Al–Si–Cu alloys

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Abstract

Quantification of precipitate fraction is difficult when the precipitates formed are of low volume fraction. A simple method is proposed in the present work to estimate the precipitate fraction of Al_2Cu phase in Al–Si–Cu alloys based on X-ray diffraction analysis. The change in the lattice parameter of the matrix due to ageing, measured from X-ray diffraction profiles, is correlated to the fraction of Al_2Cu phase formed during ageing. JMatPro, a software package for calculating the properties of metallic systems, is used to calculate the phase constitution and composition in the Al–Si–Cu alloys studied after different heat treatments. Factors that affect the lattice parameter of the matrix have been discussed and considered in the calculations.

Keywords: Precipitate fraction; Aluminium alloys; X-ray diffraction analysis; Ageing

Al–Si–Cu alloy system is of great importance in the die casting industry. The addition of Cu increases considerably the strength of Al–Si alloys, due to precipitation of a much dispersed Al_2Cu (θ') phase during ageing [1–3]. The strengthening contribution from precipitates is typically a function of both precipitate size and fraction [4,5]. Quantification of precipitation hardening therefore requires detailed knowledge of the evolution of precipitate size and fraction during ageing. There has been extensive work on precipitate type identification and size measurement [1–3,6–8], whereas little information is available on quantification of the precipitate fraction in aluminium alloys. In a recent study, a method was proposed to estimate the fraction of precipitates of nanometre scale in C250 maraging steel and has demonstrated promising results [9]. This method may also be applicable to some precipitation hardened aluminium alloys and nickel-based superalloys. In the present work, an attempt was made to apply this method to estimate the precipitate fraction in two Al–Si–Cu alloys. JMatPro (acronym for Java-based Materials Properties), a software for materials property simulation [10], has been used to calculate precipitate type and equilibrium fraction after different heat treatments. The database used in the calculation, Al-DATA, is a comprehensive thermodynamic database for Al-alloys with a proven track record [11].

Two aluminium alloys of composition Al–10Si–2Cu and Al–10Si–4Cu (numbers indicate wt.%) were chosen in the present study (their compositions in at% are Al–9.76Si–0.86Cu and Al–9.87Si–1.75Cu, respectively). The experimental work was carried out by Król [1]. The two alloys were melted and cast in argon atmosphere, directionally solidified at 28 μm/s. They were then homogenised in argon atmosphere at 530 °C for 1 h, quenched in water and aged at 200 °C. The X-ray diffraction (XRD) analysis was carried out on a conventional Philips PW 1710 diffractometer with horizontal goniometer; more experimental details can be referred to [1]. Calibration procedure and alignment were performed according to service instruction by specialized service engineer from Philips Service Poland, on the basis of the standard sample of Si. The measurements were carried out at room temperature (22 °C). This temperature was not specially stabilized but the fluctuations of the temperature were not larger than ±1 °C in the goniometer area. The matrix lattice parameter change due to this precipitation has been clearly measured through X-ray diffraction analysis

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Table 1
Volume of the alloying elements in FCC matrix

Element	Volume ($\times 10^{-6}$ m^3/mol)	Volume ($\times 10^{-29}$ m^3/cell)
Al	10	1.66113
Si	12.1	2.00997
Cu	7.1	1.17940

by Król [1]. The procedures of estimating precipitate fraction from matrix lattice parameter are briefed below.

For a matrix of an alloy having any of the 14 Bravais lattices [12], whose unit cell contains N atoms, the volume of one unit cell, V [13], can be estimated from the chemical composition of the matrix

$$V = N \times \sum_i \frac{X_i V_i}{100}$$

where X_i and V_i are the atomic percentage and the atomic volume of the ith element, respectively. Under this general formula, the matrix of aluminum alloys has a face-centred-cubic (FCC) structure, whose unit cell contains four atoms. The volume of one unit cell, V, can be estimated from the chemical composition of the matrix

$$V = a^3 = 4 \times \sum_i \frac{X_i V_i}{100} \quad (1)$$

where a is the lattice constant. When precipitates form, the composition of the matrix changes from X_i to X_i', resulting in a change of V to V' and a to a'. When a certain amount of precipitate-forming elements leaves the matrix to form precipitates, their positions are occupied by other atoms of different atomic volume. The atomic volume of different alloying elements is given in Table 1. For instance, the precipitation of Si atoms, whose atomic volume is larger than $V/4$, will result in V' smaller than V, whereas the precipitation of Cu atoms will lead to a larger V' than V. The correlation between precipitate fraction f and $a_{\text{aged}} - a_{\text{quenched}}$ can therefore be established when the precipitate type is known. Detailed procedures of this method can be referred to [9].

The Al–Si–Cu alloys studied differ from the previous work on C250 maraging steel in that the microstructure prior to ageing treatment is not a single phase, but with silicon precipitates. Phase constitution and element distribution in each phase after holding at 530 °C was calculated using JMatPro and given in Table 2. The composition of the Al-phase at 530 °C in each alloy serves as the matrix composition prior to ageing in the calculations. During the subsequent ageing at 200 °C, Al_2Cu phase precipitates out from the matrix. Due to the different amount of Cu in the original alloys, the amount of Al_2Cu formed is very different, as can be seen in Table 2.

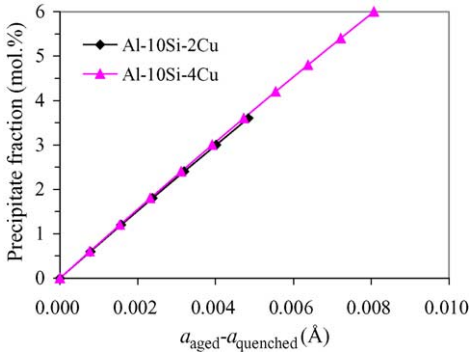

Fig. 1. Correlation between $a_{\text{aged}} - a_{\text{quenched}}$ and precipitate fraction of Al_2Cu.

Through calculation, the relation between the change in lattice parameter and the amount of precipitates formed in Al–10Si–2Cu and Al–10Si–4Cu alloys is established (Fig. 1). The values for $a_{\text{aged}} - a_{\text{quenched}}$ are positive because the lattice constant after ageing becomes larger than that in as-quenched condition due to the precipitation of small Cu atoms. The two lines are very close since the alloys have similar composition and the precipitates formed are both Al_2Cu (θ'). Also, because the amount of precipitates is small, the non-linearity of the curve is not clearly shown. By applying such relationship to the observed change in lattice parameter from XRD analysis, the evolution of precipitate fraction during ageing can be obtained.

However, the measured lattice parameter of the Al-rich matrix needs to be corrected. There are two factors that affect the lattice parameter of the Al-rich phase during ageing. One is the thermal misfit due to the difference in thermal expansion coefficient between matrix and Si precipitate. The other is the precipitation of Cu and Si atoms from the Al-rich phase during ageing. Since this paper deals with the precipitation of Cu atoms, the change in lattice parameter caused by other factors should be removed.

The microstructure after solution treatment at 530 °C is a mixture of Al-rich phase and Si particles. There exist different opinions on whether fresh Si particles precipitate out during the following ageing at around 200 °C. Starink and Mourik concluded that θ' phase and Si phase precipitation proceeds simultaneously based on their differential scanning calorimetry study [14], whereas Reif et al. observed no precipitation of Si during ageing of similar alloys [6]. It is probably difficult to observe the formation of about 1% fresh Si phase when

Table 2
Phase constitution at different temperatures in the two alloys studied

Alloy (wt.%)	Temperature (°C)	Phase constitution (mol%)
Al–10Si–2Cu	530	91.22% Al (Al–1.07Si–0.95Cu) + 8.78% Si
	200	87.77% Al (Al–0.0067Si–0.044Cu) + 9.75% Si + 2.48% Al_2Cu
Al–10Si–4Cu	530	91.17% Al (Al–1.13Si–1.88Cu) + 8.83% Si
	200	84.99% Al (Al–0.0067Si–0.044Cu) + 9.87% Si + 5.14% Al_2Cu