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Effect of Sc on the Ageing and Microstructure of an Al-Cu-Mg Alloy

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Abstract

We have studied the effect on the ageing behaviour of 0.2 wt.% addition of Sc to a base Al-2.5Cu-1.5Mg alloy. The hardening response was augmented such that peak hardness was increased ~ 12%. The decomposition was haracterized using transmission electron microscopy and simulated using a Monte Carlo calculation. The addition of Sc refines the dispersion of GPB zones and the simulation results reveal a strong tendency for Sc to cluster with vacancies and Mg atoms. These results are discussed in terms of the rapid initial hardening observed in these alloys and support the cluster hardening proposal.

1. Introduction

The intriguing capacity of certain Al-Cu-Mg alloys, possessing compositions in the α+S field of the Al-Cu-Mg phase diagram [see e.g. 1] to exhibit a very rapid initial hardening response [1] has been the subject of numerous recent studies [2, 3]. It has been shown that this initial hardening can be augmented by thermomechanical processing [4] or by alloying [5]. Microalloying with Sc in age hardenable Al alloys has also aroused increasing interest in recent years, since it has been demonstrated that small Sc additions can improve a range of mechanical properties in Al-Mg, Al-Zn-Mg and Al-Li heat treatable alloys [3]. On the basis of evidence that the mechanism of the rapid hardening behavior in Al-Cu-Mg alloys relates to solute-vacancy clusters [2-5], we have examined the effect of Sc additions to a base Al-2.5Cu-1.5Mg alloy system. The work was initiated to examine for the possibility of augmenting the hardening reaction by either stimulating extensive solute clustering or refining precipitation. A Monte Carlo (MC) approach was selected to study likely effects of Sc during the early stages of decomposition and analytical transmission electron microscopy (TEM) used to correlate microstructure and properties in this system where rather less, generally, has been published on the effects of Sc on hardening and microstructure.

2. Experimental Procedure and Simulation Model

The compositions of the alloys investigated are listed in Table 1. The ingots were homogenised, scalped, hot rolled and fabricated to sheets 2 mm thick by cold rolling, before samples were solution heat treated at 525 °C for 1 h, followed by cold water

quenching and aged at 150 °C in oil. Their age hardening response was monitored using microhardness indentation under 200 g. Specimens for TEM were electropolished using standard techniques and examined using a Philips CM12 operating at 120 kV.

Table 1: The normal compositions of the studied alloys (wt%).

Alloy	Cu	Mg	Sc	Al
A	2.5	1.5		Balance
B	2.5	1.5	0.2	Balance

A MC approach was used to provide insights into the solute-vacancy distributions during the early stages of ageing, where the opportunity for direct observations using TEM is known to be difficult. A rigid fcc lattice with 100x100x102 atoms under the periodic boundary condition was used and the movement of atoms occurred through the exchange of a randomly selected vacancy with one of its nearest neighbor atoms when the transition probability, w, was greater than a randomly number, x, where 0≤x≤1. The value of w was calculated from the symmetrical solution to:

$$w = \frac{\exp(-dE/kT)}{1+\exp(-dE/kT)} \quad (1)$$

where k is Boltzman's constant, T the simulation temperature and dE the difference in total cohesive energy between atomic configurations before, E_{before}, and after, E_{after}, the exchange, such that:

$$dE = E_{after} - E_{before} = (\sum \varepsilon_{v(j)i} + \sum \varepsilon_{j(v)i'}) - (\sum \varepsilon_{v(v)i} + \sum \varepsilon_{j(j)i'}) \quad (2)$$

Here, $\sum \varepsilon_{v(j)i}$ is the sum of cohesive energy between the vacancy at the position of the j_{th} atom and its nearest atoms after the exchange; $\sum \varepsilon_{j(v)i'}$ the sum of cohesive energy between the j_{th} atom at the position of the vacancy and its nearest atoms after the exchange; $\sum \varepsilon_{v(v)i}$ is the sum of cohesive energy between the vacancy at its own position and the nearest atoms before the exchange and $\sum \varepsilon_{j(j)i'}$ the sum of cohesive energy between the j_{th} atom at its own position and its nearest atoms before the exchange. The interaction energy parameters used for the MC calculations were partly taken from Hirosawa et al. [6] as summarised in Table 2. No less than three MC runs were used.

Table 2: Interaction Energy Parameters (kJ/mol).

	Al	Cu	Mg	Sc	Vacancy
Al	-54.5	-49.3	-34.5	-47.25	-21.9
Cu		-48.5	-32.2	-42.41	-19.3
Mg			-16.8	-36.5	-10.3
Sc				-35.5	-25.8
Vacancy					2.3

3. Results

3.1 Age Hardening Response:

Figure1 indicates that both alloys exhibit similar trends in age hardening responses; hardening occurs in two distinct stages, the first of which is very rapid and the second of

which leads to peak hardness after ~ 600 h ageing. These two hardening stages are separated by an incubation period of ~ 100 h during which the hardness remains almost constant. There is a very slight increase in the initial rapid hardening in the Sc-containing alloy and this slight differential in hardness increases gradually through the second stage of hardening resulting in a peak hardness ~ 12% higher than the base alloy.

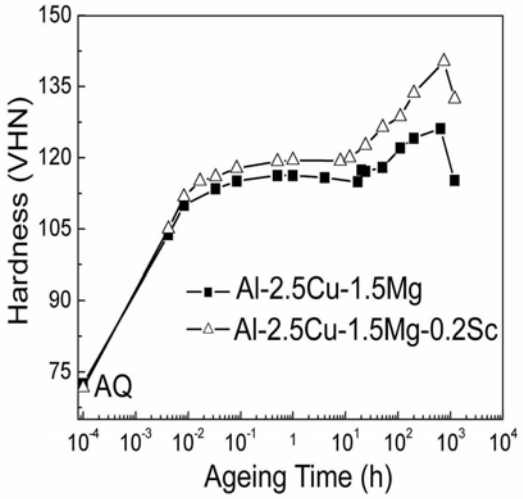

Figure 1: Hardness-time curve for the Al-2.5Cu-1.5Mg-(0.2Sc) alloys aged at 150℃. AQ:as quenched.

3.2 Simulation Results:

Figures 2(a) and (b) are two-dimensional atomic configurations from a single random $\{001\}_\alpha$ plane from the base and the Sc-containing alloy, respectively, following $8x10^8$ MC steps which we estimate corresponds to the order of a few seconds of ageing. In addition to Mg-Cu-vacancy complexes, numerous Cu-Mg co-clusters form in the base alloy. Alternatively, Sc-Mg-vacancy complexes form in the Sc-containing alloy, which occasionally contained Cu, together with Mg-Sc-Cu co-clusters and Mg-Sc co-clusters. Relatively few Cu-Sc co-clusters were observed. Figures 3(a) and (b) graph the mean size of clusters involving Cu atoms and those involving Mg atoms, respectively, as a function of the number of MC steps. This data confirm that Cu clustering is suppressed, whereas Mg clustering is stimulated by the addition of Sc. We have also calculated the probability of solute atoms positioned adjacent to Sc atoms, Figure 4(a), and adjacent to vacancies, Figure 4(b), for the Sc-containing alloy. The affinity between Sc and Mg is demonstrated in Figure 4(a), whereas the Sc-Cu interaction remains low. The most common solute interaction with vacancies is from Mg followed by Sc: both exhibit a strong and increasing interaction. There is little probability for Cu atoms to segregate to vacancies in this alloy.

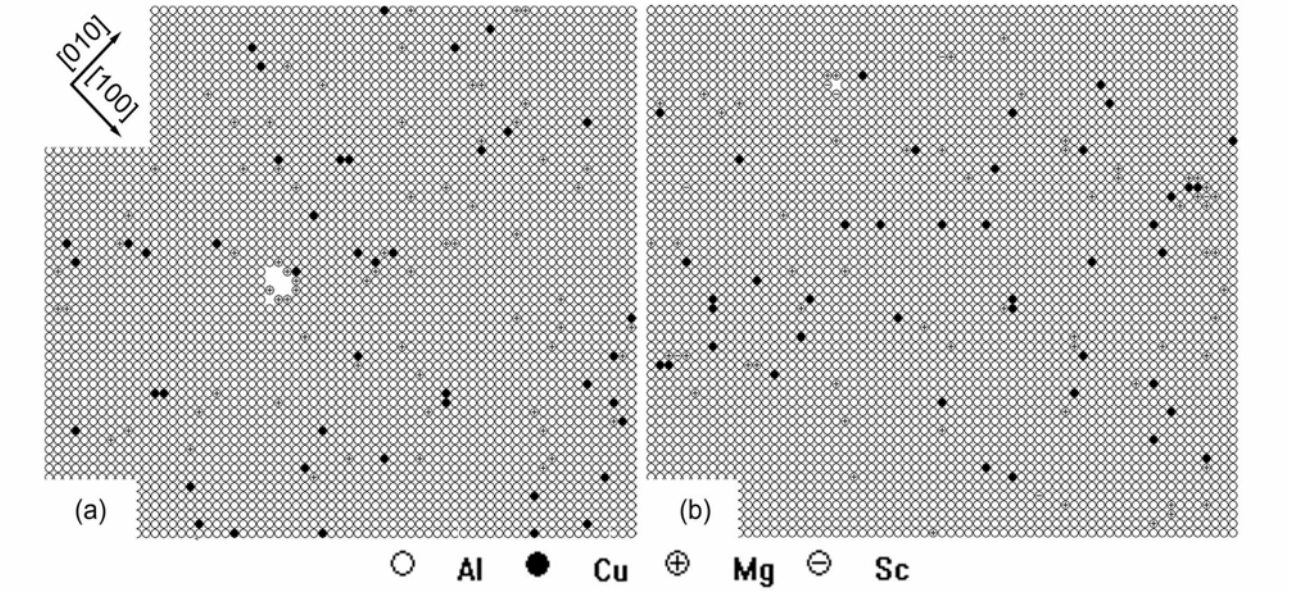

Figure 2: Typical atom configuration from a random {001}$_\alpha$ plane in (a) Al-2.5Cu-1.5Mg and (b) alloy containing 0.2Sc,calculated after 8×10^8MC steps.

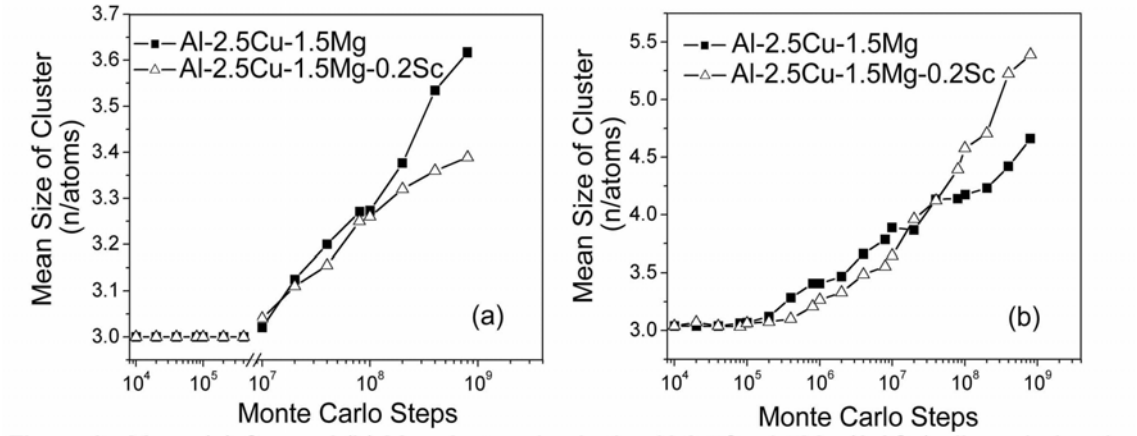

Figure 3: Mean (a) Cu- and (b) Mg- cluster size in the Al-2.5Cu-1.5Mg-(0.2Sc) alloys during the initial ageing stage.

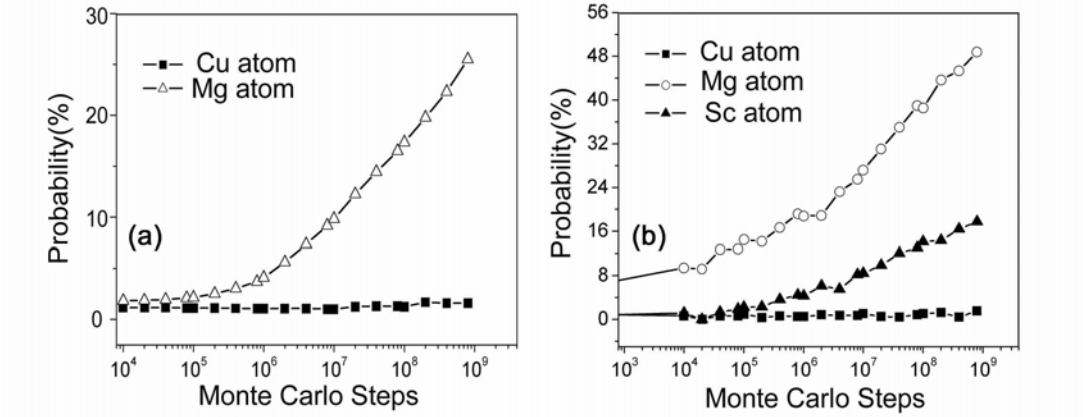

Figure 4: Probability of solute atoms positioned adjacent to (a) Sc atoms and (b) vacancies in the Al-2.5Cu-1.5Mg-0.2Sc alloys during the initial ageing stage

3.3 Electron Microscopy

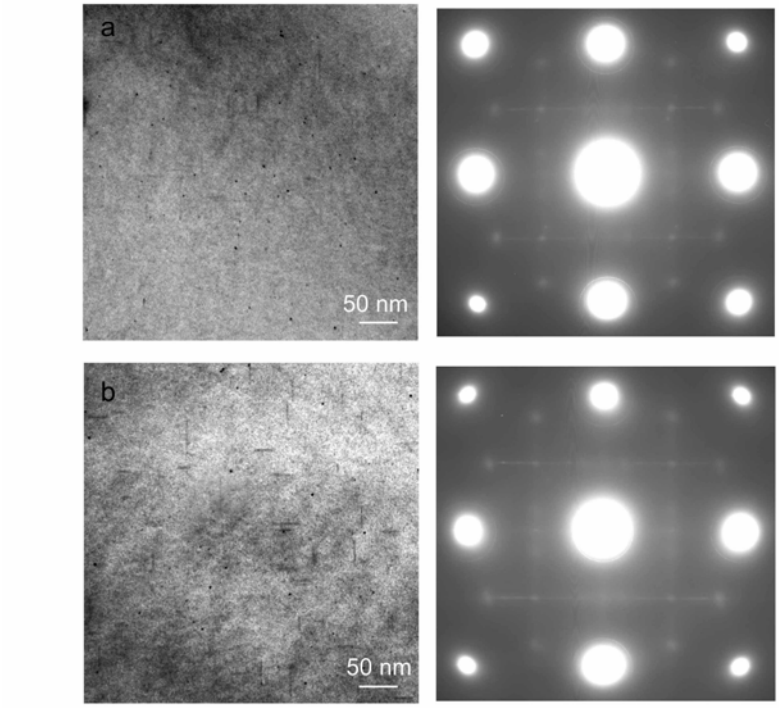

Figure 5: <001>$_\alpha$ BF TEM images and corresponding SAED patterns of (a) Al-2.5Cu-1.5Mg and (b) Al-2.5Cu-1.5Mg-0.2Sc after ageing at 150℃ for 91h.

Figure 5(a-d) are typical TEM images and selected area electron diffraction (SAED) patterns following ageing for 91 h at 150 °C: the end of the hardness plateau, Figure 1. The bright field (BF) images reveal rod-shape precipitates oriented along <100>$_\alpha$ directions. The SAED patterns exhibit diffuse streaking through {100}$_\alpha$ along <100>$_\alpha$directions with extra intensity near the {100}$_\alpha$ positions. These results are consistent with GPB 〔 zone formation. The Sc-containing alloy contains a significantly more uniform dispersion of GPB zones in this underaged condition. Following ageing for 638 h, Figure 6, GPB zones together with S phase (Al_2CuMg) dominate the microstructure of both alloys. Again, the precipitate dispersion in the Sc-containing alloy is finer and more uniform.

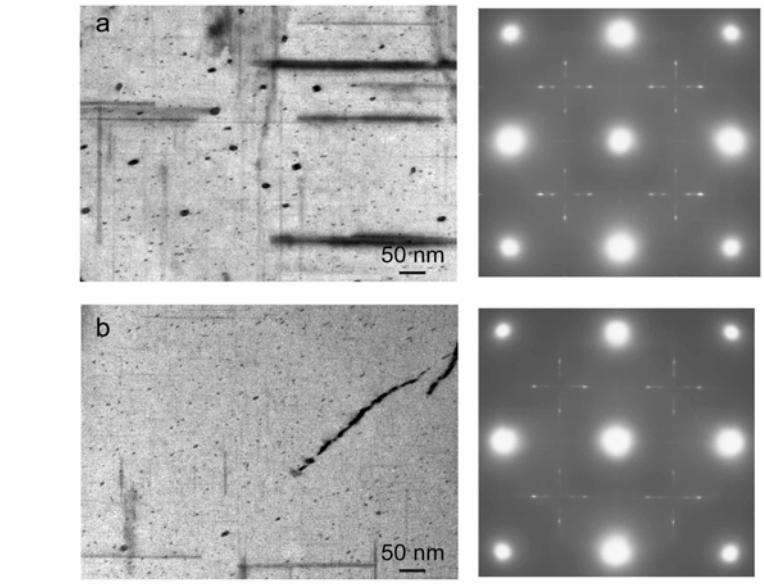

Figure 6: <001>$_\alpha$ BF TEM images and corresponding SAED patterns of (a) Al-2.5Cu-1.5Mg and (b) Al-2.5Cu-1.5Mg-0.2Sc after ageing at 150℃ for 638h.

4. Discussion

This work demonstrates that the general form of the ageing curves of the Al-2.5Cu-1.5Mg is not altered by microalloying with Sc. However, the Sc addition enhances the age hardening response, particularly the second stage of hardening. The higher peak hardness is attributed to the higher number density of precipitates in the Sc-bearing alloy. This is attributed to the cluster-stimulated nucleation of GPB zones and S phase following the more extensive formation of pre-precipitate solute co-clusters in this alloy. Early work [e.g. 7] proposed that the first stage of hardening in α+S Al-Cu-Mg alloys was due to the precipitation of GPB zones and that the second stage due to precipitation of the S phase [2]. More recently, it was proposed that the initial rapid hardening was due to co-clustering of Cu-Mg atoms and subsequently Reich et al [4] showed the significance of solute-dislocation interactions. This calculations reported in this work reveal that there exists an abundance of atomic co-clusters in both the Sc-free and Sc-containing alloys during the initial stages of ageing and suggests that the cluster-hardening mechanism is highly plausible, especially since there is no evidence of precipitation during the first few tens of seconds of ageing. The ability of clusters to strengthen alloys is becoming well established experimentally, using 3DAP methods [e.g. 8] and this has also been described by Haasan [9]. It is proposed that the strengthening arises from the extra energy required for dislocations to cut diffuse antiphase boundaries formed by the pairing (or higher order combinations) of the clustered solute species.

5. Conclusion

Microalloying of 0.2 wt. % Sc to Al-2.5Cu-1.5Mg causes:

(a) no change to the two-stage form of the hardening reaction but increases the overall response, particularly the second stage;
(b) enhanced atomic clustering such that there is a strong tendency to form Mg-Sc-vacancy complexes and Mg-Sc co-clusters;
(c) a refinement in the dispersion of GPB zones and S-phase precipitates;

As a result, we conclude that the rapid initial hardening is due to the formation of clusters and that the enhanced precipitation of GPB zones and S-phase in the Sc-containing alloy is a result of cluster-assisted nucleation from the higher number density of these clusters.

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