## Introduction

Aluminium alloys with scandium (Sc) addition have excellent mechanical properties at room temperature, due to the presence of coherent, nanometer size Al<sub>3</sub>Sc precipitates that can be obtained at a very high number density. Al<sub>3</sub>Sc has a Al<sub>3</sub>M\_L1<sub>2</sub> structure that can be stable at very high temperatures, even above liquidus. It can stabilize a fine-grain structure and also serve as a strengthening phase that blocks mobile dislocations [1]. The thermodynamic description of Al<sub>3</sub>Sc has already been included in the previous versions of JMatPro®. This report describes an improvement in JMatPro® Ver. 14, by considering the precipitation kinetics and strengthening of Al<sub>3</sub>Sc and its effect on the age hardening curve of aluminium alloys. Validation against experimental data is provided and the application range of Sc addition is discussed.

# Comparison between Al<sub>3</sub>Li and Al<sub>3</sub>Sc

Unlike lithium (Li), which can form a more commonly known  $Al_3M_Ll_2$  phase of  $Al_3Li$  in many commercial aluminium alloys such as AA2198 and AA8090, addition of Sc and its industrial application has been less established, partly due to the high cost of Sc. Here we firstly compare between  $Al_3Li$  and  $Al_3Sc$  to provide insights of the new strengthening phase  $Al_3Sc$ .

Both phases have been reported to be coherent ordered phases with nearly spherical shape [2,3], thus can induce the order strengthening effect. Al<sub>3</sub>Li is a metastable strengthening phase that eventually transforms into its stable counterpart ALLI, whereas Al<sub>3</sub>Sc remains stable at elevated temperatures, as depicted in the equilibrium phase distribution of an example ternary Al-Li-Sc alloy in Fig. 1.



Fig. 1 Equilibrium phase distribution of an example ternary Al-Li-Sc alloy

Sc diffuses ~1000 times slower than Li so the kinetics of Al<sub>3</sub>Sc formation is much slower than that of Al<sub>3</sub>Li. Although Sc and Li can co-exist in Al<sub>3</sub>M\_L1<sub>2</sub>, they are favoured in different temperature ranges with Al<sub>3</sub>Sc being a high temperature strengthening phase and Al<sub>3</sub>Li a low temperature strengthening phase. In the calculated phase composition of Al<sub>3</sub>M\_L1<sub>2</sub> of the ternary Al-Li-Sc alloy shown in Fig. 2, it can be seen that Sc dominates Al<sub>3</sub>M\_L1<sub>2</sub> when the temperature is above 200°C.



Fig. 2 Phase composition of Al<sub>3</sub>M\_L1<sub>2</sub> of a ternary Al-Li-Sc alloy

Furthermore,  $Al_3Sc$  has comparatively higher interfacial energy and larger lattice parameter mismatch than  $Al_3Li$  with respect to the aluminium matrix, so that  $Al_3Sc$  has a higher coherency hardening effect than  $Al_3Li$ .

# Modelling the transformation kinetics of Al<sub>3</sub>Sc

The original Johnson-Mehl-Avrami (JMA) theory is used to describe the nucleation and growth of Al<sub>3</sub>Sc [4] and Lifshitz-Slyozov-Wagner (LSW) theory is used to model the coarsening of Al<sub>3</sub>Sc [5]. In both theories, an effective diffusivity is considered, which is composed of lattice diffusivity and dislocation pipe diffusivity. Here the rate-controlling element is solely Sc due to its very slow diffusivity. Fig. 3(a-b) provides two example comparisons between the calculated and measured evolution of the average radius of spherical Al<sub>3</sub>Sc particles in two ternary Al-Mg-Sc alloys, subjected to different ageing temperatures. Good agreement is achieved and note that all the ageing temperatures are relatively high compared with that of conventional aluminium alloys.



Fig. 3 Comparison between calculated and measured evolution of  $Al_3Sc$  particle radius of (a) Al-2Mg-0.2Sc (wt%) [6] and (b) Al-1Mg-0.27Sc (wt%) [7], at different ageing temperatures.

When Zr is added in conjunction with Sc to aluminium alloys, a phenomenological "core-shell" structure has been frequently observed, where Al<sub>3</sub>Sc nucleates first as the core and Al<sub>3</sub>Zr gradually diffuses towards Al<sub>3</sub>Sc, forming a shell surrounding Al<sub>3</sub>Sc and hindering the coarsening of the core as Zr diffuses much slower than Sc [8,9]. To reflect these characteristics in the kinetics modelling, when a notable amount of Zr is added, the rate-controlling element switches from Sc during nucleation and growth to Zr during subsequent coarsening.

## Modelling the strengthening effect of Al<sub>3</sub>Sc

Like other ordered phases, such as Al<sub>3</sub>Li in aluminium, and  $\gamma'$  phase in Ni-based superalloys, the first and foremost strengthening effect is the order strengthening mechanism, i.e. dislocations overcoming ordered particles by shearing or cutting. These dislocation-precipitate interaction modes have been characterised into two stages, respectively weak and strong dislocation pair coupling [10-12], which effectively depict a transition in strength evolution depending on the size of particles and the number of dislocations that can reside in one particle [13].

Further, similar to the scenario of  $\gamma$ " phase in Ni-based superalloys [14,15], a coherency strengthening effect is considered here for Al<sub>3</sub>Sc due to the relatively large lattice mismatch compared with Al<sub>3</sub>Li [16]. As the particles grow significantly in size, the Orowan looping mechanism becomes predominant [17], in which dislocations bypass particles by punching out loops and thereafter the coherency of the particles is lost.

### Evaluating the age hardening curves of Sc-containing alloys

In this section, comparisons between the calculated and measured age hardening curves of some binary Al-Sc and ternary Al-Sc-X alloys ('X' represents an additional type of element) are presented to validate the proposed approach. Note that all the original measurements are in the format of Vickers hardness. The JMatPro® internal conversion tool was used to convert the calculated yield strength into hardness for comparison. Fig. 4 presents the age hardening curves of two binary Al-Sc alloys with cast T6 conditions. Both alloys were homogenized at ~640°C, followed by water-quenching but subsequently different ageing temperatures. Good agreement is achieved in accordance to the general trend such that with the increase of temperature, the transformation accelerates and the peak strength is obtained faster.



Fig. 4 Evolution of hardness with different ageing temperatures for Al-0.3Sc (wt%) [3] and Al-0.18Sc (wt%) [18] alloys at cast T6 conditions. The initial homogenization temperature was 648°C for Al-0.3Sc and 640°C for Al-0.18Sc.

Figures 5 and 6 compare the age hardening curves between binary Al-Sc alloys and ternary Al-Sc-X alloys with Mg or Ni addition, all at the ageing temperatures of 300°C and 350°C. While the age hardening curve can shift up with additional Sc (Fig. 6) because of an increase in the fraction of Al<sub>3</sub>Sc during ageing, the addition of Mg and Ni also contribute to the strength increase (~20-40 Hv) due to the additional solid solution strengthening effect. It is also noted that an addition of Sc can make the binary Al-Mg or Al-Ni alloys heat-treatable, as otherwise the age hardening curves without Sc would be rather flat [20].



Fig. 5 Age hardening curves of binary Al-0.2Sc (wt%) and ternary Al-2Mg-0.2Sc (wt%) alloys at cast T6 condition [19]. The alloys were homogenized at 617°C, quenched into room temperature and subsequently aged at 300°C and 350°C.



Fig. 6 Age hardening curves of binary Al-0.2Sc (wt%), Al-0.4Sc (wt%) and ternary Al-6Ni-0.2Sc (wt%), Al-6Ni-0.4Sc (wt%) alloys at cast T5 condition [20], with the ageing temperature of 300°C and 350°C.

Figure 7 shows the age hardening curves of two Al-Sc and Al-Sc-Zr alloys, demonstrating the effect of the aforementioned core-shell structure. In Fig. 7(a), the dashed line represents the age hardening behaviour of the ternary Al-Sc-Zr alloy if the coarsening is controlled by Sc rather than Zr, for a comparison with the solid red line where the coarsening is controlled by Zr. The good agreement clearly shows that an addition of Zr can provide resistance to coarsening by slowing down the strength reduction.



Fig. 7 Comparison of the age hardening curves between (a) binary Al-0.4Sc (wt%) and ternary Al-0.4Sc-0.15Zr (wt%) alloys [21]; (b) binary Al-0.3Sc (wt%) and ternary Al-0.3Sc-0.09Zr (wt%) alloys [22] at cast T5 condition with the ageing temperature of 350°C.

### **Application range**

From the results shown above, it is observed that just a small amount of Sc (~0.2-0.4 wt%) can provide a considerable strengthening effect, with a maximum increase of Vickers hardness around 50-60 Hv (or ~100-130 MPa yield strength) when aged at elevated temperatures. In fact, many studies on the effect of Sc have used materials with no more than 0.6 wt% of Sc. A few studies with much higher amount of Sc have shown no significant additional benefit to the strength compared with lower amount of Sc [23,24]. This demonstrates that the amount of Sc that can be precipitated from supersaturated solid solution is rather limited [25]. One explanation for this is that, as Al<sub>3</sub>Sc is a stable phase at elevated temperatures even in liquid state (Fig. 1), excessive Sc may be 'wasted' by the initial heat treatment due to the formation of pre-existing stable large particles of Al<sub>3</sub>Sc before commencement of any ageing treatment.

Further, Fig. 2 shows that, in all different types of Al<sub>3</sub>M\_L1<sub>2</sub> phase, Sc only dominates at relatively high temperatures. This illustrates that the temperature regime for age hardening by precipitation of Al<sub>3</sub>Sc is somewhere in between the temperature regimes for conventional age hardening and solution heat treatments of common precipitation hardened alloys. This makes a combined precipitation of Al<sub>3</sub>Sc and other strengthening precipitates unfeasible. Therefore, precipitation strengthening by Al<sub>3</sub>Sc is most feasible in alloy systems that are non-heat-treatable, such as 1xxx, 3xxx and 5xxx [25]. Some additional yield strength (YS) results in these alloy systems are calculated and compared in Table 1, with most of the experimental work on Sc on 1xxx-types of alloys carried out on binary Al-Sc alloys with much higher purity than industrial alloys. References of these data can be found in [25].

System	Composition, wt%	YS, MPa (exp)	YS, MPa (cal)	Note
1xxx	0.1Sc	132	120	Wrought, quenched from 630°C, aged 320°C/13.3h
	0.2Sc	138	142	Cast T5, aged 300°C/10h
	0.23Sc	159	161	Cast T5, aged 288°C/8h
	0.38Sc	199	193	Cast T5, aged 288°C/8h

Table 1 Yield strength in some non-heat-treatable Al-alloys with Sc

	0.4Sc	196	198	Cast T5, aged 300°C/10h
	0.5Sc	160	149	Wrought, quenched from 649°C, aged 288°C/8h
3xxx	0.5Mg, 0.2Mg, 0.26Sc, 0.15Zr	162	155	Wrought, solutionised 600°C, aged 250°C/1000h
5xxx	4Mg, 0.2Sc	194	199	Cast T5, aged 300°C/10h

#### Summary

Compared with common Al<sub>3</sub>M\_L1<sub>2</sub> phases such as Al<sub>3</sub>Li, Al<sub>3</sub>Sc is a highly stable phase even at supersolvus temperature. The transformation kinetics of Al<sub>3</sub>Sc and its strengthening effect during artificial ageing of aluminium alloys have been evaluated and incorporated in JMatPro® Ver. 14. Besides the conventional order strengthening and Orowan looping mechanisms and their transition, the coherency strengthening effect is also considered due to the relatively large lattice mismatch of Al<sub>3</sub>Sc. A phenomenological core-shell structure of Al<sub>3</sub>Sc/Al<sub>3</sub>Zr is also taken into account where an addition of Zr provides resistance to coarsening.

The approach has been validated by good agreement with the measurement of age hardening curves of Sccontaining binary and ternary alloys in literature with different amount of Sc. It captures the fact that a small amount of Sc can provide notable enhancement of strength. Note that as the age hardening regime of  $Al_3Sc$ is much higher than that of common precipitation hardened alloys, the traditionally non-heat-treatable aluminium alloy systems would benefit more from the addition of Sc. Considering the high cost of Sc in practice [26], the improvement in this work could economically assist the design and assessment of the addition of Sc in the aluminium industry.

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