Thermal expansion of Al₃Sc and Al₃(Scₓ₀.₇₅X₀.₂₅)

Y. Harada a, D.C. Dunand b, *

a Institute of Mechanical Systems Engineering, National Institute of Advanced Industrial Science and Technology, 1-2-1 Namiki, Tsukuba, Ibaraki 305-8564, Japan
b Department of Materials Science and Engineering, 2220 Campus Drive, Northwestern University, Evanston, IL, 60208, USA

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Abstract

The thermal expansion coefficient of Al₃Sc and Al₃(Scₓ₀.₇₅X₀.₂₅), where X is Ti, Y, Zr or Hf, was measured by dilatometry between 25 and 1000 °C. The measured value, (16 ± 1) × 10⁻⁶ K⁻¹, is constant between 25 and 900 °C and insensitive to alloying element. Good agreement is found with a literature value determined from first-principle calculations.

Keywords: Intermetallic compound; Aluminum alloys; Thermal expansion; Scandium

1. Introduction

A few tenths of wt.% alloying addition of scandium to aluminum markedly enhances strength at ambient and elevated temperature by the precipitation of coherent, nano-size Al₃Sc precipitates with the cubic L₁₂ structure [1], which interact strongly with matrix dislocations [2]. Because of the low solubility and diffusivity of Sc in Al, and the small lattice mismatch between Al₃Sc and Al, the coarsening rate of Al₃Sc precipitates in Al is very low up to 300 °C [3,4], and can be further reduced by the formation of a solid solution, e.g., Al₃(Sc,Zr) [1,5]. This low coarsening rate allows for the use of coarse-grained Sc-containing aluminum alloys under creep conditions at temperature as high as 350 °C, where the interaction of matrix dislocations with the precipitates leads to a threshold stress, below which dislocation creep is not measurable [2,6]. Recently, it has been shown that the threshold stress increases with precipitate radius, an unexpected finding that was modeled by considering the elastic interaction between dislocations and precipitates [2,7]. The main prediction of this model is that this elastic interaction (and thus the threshold stress) increase with increasing lattice mismatch between the matrix and precipitates. This mismatch should however be minimized to improve coarsening resistance. A careful tailoring of the lattice mismatch between matrix and precipitates is thus necessary at the use temperature, which is possible only if the coefficient of thermal expansions (CTEs) of Al₃Sc and its solid solutions (e.g., Al₃(Sc,Zr)) are known, since the thermal expansion mismatch is expected to significantly affect the net lattice mismatch at elevated temperature. The purpose of the present note is to report experimental measurements of the CTE for...
binary Al₃Sc and ternary Al₃(ScₓTi₁₋ₓ) intermetallics, where X is Ti, Y, Zr or Hf.

2. Experimental procedures

Buttons of binary Al₃Sc and ternary Al₃(ScₓTi₁₋ₓ) were produced by non-consumable electrode arc-melting of 3–5 g pure elements (99.99% Al, 99.94% Sc, 99.999% Ti, 99.9% Y, 99.94% Zr and 99.97% Hf) on a water-cooled copper hearth under a purified, titanium-gettered argon atmosphere. Melting of the button was performed four or more times, flipping the button after each solidification to ensure complete mixing of the metals. Every button was subsequently homogenized in vacuum (10⁻⁴ Pa) for 2 h at 1200 °C. Electro-discharge machining was used to create cylindrical specimens with 4 mm diameter and 8 mm length for binary Al₃Sc and ternary Al₃(Sc₇₅Zr₂₅), reduced to 3 and 6 mm, respectively, for the other ternary alloys. The longitudinal direction of these specimens was aligned with the vertical direction of the arc-melted button, corresponding to the main solidification direction, along which large grain (∼0.5–1 mm) were oriented.

CTE measurements were performed in a dilatometer (Thermo Mechanical Analyzer TMA-50, Shimadzu) using quartz push-rod and boat. The temperature was increased from 25 to 1000 °C at a rate of 5 K/min. Repeatability was verified by measuring each specimen three times, from which an experimental error of ±1 × 10⁻⁶ K⁻¹ was estimated. Measurements were performed under mechanical-pump vacuum which was sufficient to prevent oxidation, as verified by measuring negligible mass changes after the experiments.

3. Results and discussion

Fig. 1 shows the dilatometric curve for binary Al₃Sc, which exhibits an average CTE of 16.0 × 10⁻⁶ K⁻¹ between 25 and 900 °C. Al₃Sc, they report a value of 43 × 10⁻⁶ K⁻¹ for the high-temperature coefficient of volume thermal expansion (due to a mislabeling, Fig. 9 in [8] applies to AlSc, not Al₃Sc [9]). The corresponding CTE of 14 × 10⁻⁶ K⁻¹ is in satisfactory agreement with our experimental value, and lends credence to the validity of the first-principle calculations presented in [8] for elastic, thermal and thermodynamic properties in the Al–Sc system.

Fig. 2 summarizes the average CTE values for the binary and ternary alloys for the ranges 25–300, 300–600, 600–900 and 900–1000 °C. Values for the 900–1000 °C range are not reported for Al₃(Sc₇₅Zr₂₅) and Al₃(Sc₇₅Y₂₅), as they were found to be erratic (∼23 × 10⁻⁶ and 8.8 × 10⁻⁶ K⁻¹, respectively), probably because of the presence of low-melting eutectic phase leading to localized melting of Al. Fig. 2 shows that the CTE of binary Al₃Sc is not affected by the substitution of a quarter of the Sc by group IIIIB (Y) or IVB (Ti, Zr, Hf) elements; this is expected, as these elements are in solid solution within Al₃Sc at this concentration, so that all specimens show the same L₁₂ structure, with almost the same lattice parameter: 

Al₃Sc: 0.4103 nm; Al₃(Sc₇₅Ti₂₅): 0.4075 nm; Al₃(Sc₇₅Y₂₅): 0.4138 nm; Al₃(Sc₇₅Zr₂₅): 0.4095 nm; Al₃(Sc₇₅Hf₂₅): 0.4091 nm [10].
indicates that, for all specimens, the CTE does not vary between 25 and 900 °C, within the experimental error of ±1 × 10⁻⁶ K⁻¹.

Little experimental data exist on the CTE of other tri-aluminide intermetallics, with only two binary compounds listed in the standard compilation work by Touloukian et al. [11]: Al₃U with an average CTE of 15.9 × 10⁻⁶ K⁻¹ between 20 and 727 °C, and Al₃Fe with an average CTE of 14.9 × 10⁻⁶ K⁻¹ between 20 and 577 °C. Furthermore, the CTE of (Al₀.₈₉Cr₀.₁₁)₃Ti (Al–8Cr–25Ti) was reported as 15.6 × 10⁻⁶ K⁻¹ between 20 and 1000 °C [12]. All values are within the range of (16 ± 1) × 10⁻⁶ K⁻¹ measured for Al₃Sc. We note that Al₃U, (Al₀.₈₉Cr₀.₁₁)₃Ti and Al₃Sc share the same L1₂ crystal structure and have very similar melting points (1350, 1350 and 1320 °C, respectively), so that a similar CTE is indeed expected. Conversely, the CTE of Al₃Nb, which has a different DO₂₂ structure and a much higher melting point of 1680 °C, was reported as 9.6 × 10⁻⁶ K⁻¹ between 20 and 1000 °C [13].

For high-temperature structural use of aluminum alloys strengthened with nano-size, coherent Al₃(Sc,X) precipitates, a compromise must be

found between coarsening resistance and inherent creep resistance. On the one hand, optimal creep resistance is predicted, at a given precipitate size, to increase with increasing mismatch as a result of elastic interactions between dislocations and particles [7]. On the other hand, coarsening is expected to accelerate with higher lattice mismatch, with a concomitant decrease in creep resistance, due to a drop in the Orowan stress. Scandium-containing aluminum alloys for high-temperature applications may thus need to be carefully designed for an optimal lattice mismatch between the Al₃(Sc,X) precipitates and the matrix, for which the present measurements of CTE are useful.

The mismatch in lattice parameter between Al and Al₃Sc is 1.34% at ambient temperature, assuming no residual stresses and taking lattice parameter values of 0.4049 and 0.4103 nm for Al and Al₃Sc, respectively [10,14]. Given the larger CTE and smaller lattice constant of Al as compared to Al₃Sc, the mismatch decreases with increasing temperature. The lattice mismatch between Al and the binary and ternary Al₃Sc phases studied here is plotted in Fig. 3 between

![Fig. 2. Summary of experimental CTE values for binary Al₃Sc and ternary Al₃(Sc₀.₇₅X₀.₂₅).](image)

![Fig. 3. Calculated lattice mismatch between Al and Al₃Sc or Al₃(Sc₀.₇₅X₀.₂₅) as a function of temperature.](image)
25 and 600 °C, using the temperature-dependent CTE of Al [11], the average CTE values from Fig. 2 for Al$_3$Sc and Al$_3$(Sc$_{0.75}$X$_{0.25}$), and the lattice parameters of these phases at ambient temperature listed above [10]. It is evident from Fig. 3 that temperature has a significant effect on the magnitude of the lattice mismatch: at 300 °C, for example, the mismatch decreases by a factor 1.14–1.59, as compared to ambient temperature value. At a given temperature, reduction of mismatch can be achieved most efficiently by Ti additions: forming Al$_3$(Sc$_{0.75}$Ti$_{0.25}$) more than halves the lattice mismatch at 300°C, as compared to Al$_3$Sc (Fig. 3). On the other hand, Y additions can increase the mismatch by, e.g., almost a factor 2 for Al$_3$(Sc$_{0.75}$Y$_{0.25}$) at 300 °C. This effect can however be reduced by alloying the matrix with magnesium, which reduces the lattice constant of Al by 0.13% for each wt.% Mg [15].

4. Conclusions

The CTE for binary Al$_3$Sc and ternary Al$_3$(Sc$_{0.75}$X$_{0.25}$), where X is Ti, Y, Zr or Hf, was measured by dilatometry as $(16 \pm 1) \times 10^{-6}$ K$^{-1}$. This value is constant between 25 and 900 °C and insensitive to alloying additions. Good agreement is found with a literature value of $14 \times 10^{-6}$ K$^{-1}$ calculated from first principles for Al$_3$Sc, and with published CTE values for other L1$_2$ tri-aluminides. CTE values for Al$_3$Sc and Al$_3$(Sc$_{0.75}$X$_{0.25}$) are useful for the calculation of lattice mismatch in Sc-containing precipitation-strengthened aluminum alloys, which controls coarsening and creep resistance.

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