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Thermal expansion of Al_3Sc and $\text{Al}_3(\text{Sc}_{0.75}\text{X}_{0.25})$

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Abstract

The thermal expansion coefficient of Al_3Sc and $\text{Al}_3(\text{Sc}_{0.75}\text{X}_{0.25})$, where X is Ti, Y, Zr or Hf, was measured by dilatometry between 25 and 1000 °C. The measured value, $(16 \pm 1) \times 10^{-6} \text{ K}^{-1}$, 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.

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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 Al_3Sc precipitates with the cubic L1_2 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 Al_3Sc and Al, the coarsening rate of Al_3Sc 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., $\text{Al}_3(\text{Sc,Zr})$ [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 Al_3Sc and its solid solutions (e.g., $\text{Al}_3(\text{Sc,Zr})$) 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

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binary Al_3Sc and ternary $\text{Al}_3(\text{Sc}_{0.75}\text{X}_{0.25})$ intermetallics, where X is Ti, Y, Zr or Hf.

2. Experimental procedures

Buttons of binary Al_3Sc and ternary $\text{Al}_3(\text{Sc}_{0.75}\text{X}_{0.25})$, 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 Al_3Sc and ternary $\text{Al}_3(\text{Sc}_{0.75}\text{Zr}_{0.25})$, 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 $\pm 1 \times 10^{-6} \text{ K}^{-1}$ 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 Al_3Sc , which exhibits an average CTE of $16.0 \times 10^{-6} \text{ K}^{-1}$ between 25 and 900 °C, increasing to $17.7 \times 10^{-6} \text{ K}^{-1}$ between 900 and 1000 °C. Asta and Ozolins [8] recently presented first-principle calculations of the thermodynamic and physical properties of Al–Sc intermetallic compounds. For

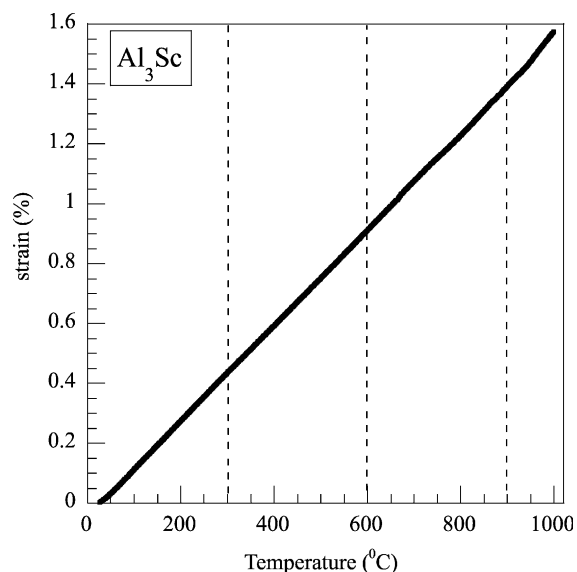


Fig. 1. Dilatometric curve for Al_3Sc showing a near constant CTE of $16.0 \times 10^{-6} \text{ K}^{-1}$ between 25 and 900 °C.

Al_3Sc , they report a value of $43 \times 10^{-6} \text{ K}^{-1}$ for the high-temperature coefficient of volume thermal expansion (due to a mislabeling, Fig. 9 in [8] applies to AlSc, not Al_3Sc [9]). The corresponding CTE of $14 \times 10^{-6} \text{ K}^{-1}$ 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 $\text{Al}_3(\text{Sc}_{0.75}\text{Zr}_{0.25})$ and $\text{Al}_3(\text{Sc}_{0.75}\text{Y}_{0.25})$, as they were found to be erratic ($\approx 23 \times 10^{-6}$ and $8.8 \times 10^{-6} \text{ K}^{-1}$, 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 Al_3Sc is not affected by the substitution of a quarter of the Sc by group IIIB (Y) or IVB (Ti, Zr, Hf) elements; this is expected, as these elements are in solid solution within Al_3Sc at this concentration, so that all specimens show the same L1_2 structure, with almost the same lattice parameter: Al_3Sc : 0.4103 nm; $\text{Al}_3(\text{Sc}_{0.75}\text{Ti}_{0.25})$: 0.4075 nm; $\text{Al}_3(\text{Sc}_{0.75}\text{Y}_{0.25})$: 0.4138 nm; $\text{Al}_3(\text{Sc}_{0.75}\text{Zr}_{0.25})$: 0.4095 nm; $\text{Al}_3(\text{Sc}_{0.75}\text{Hf}_{0.25})$: 0.4091 nm [10]. Fig. 2 also

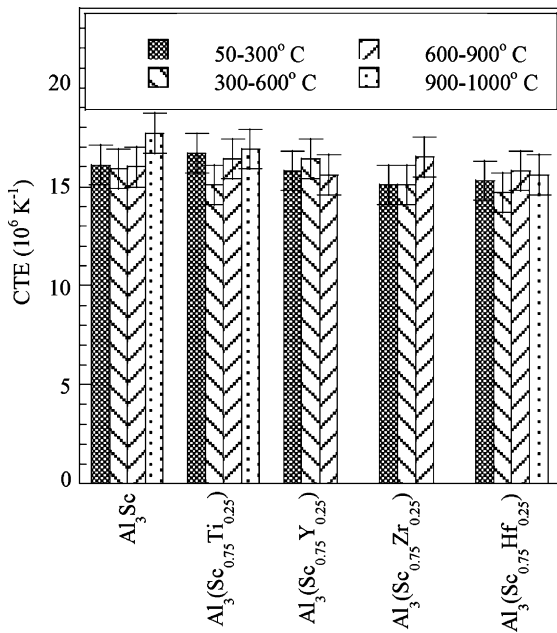


Fig. 2. Summary of experimental CTE values for binary Al_3Sc and ternary $\text{Al}_3(\text{Sc}_{0.75}\text{X}_{0.25})$.

indicates that, for all specimens, the CTE does not vary between 25 and 900 °C, within the experimental error of $\pm 1 \times 10^{-6} \text{ K}^{-1}$.

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]: Al_3U with an average CTE of $15.9 \times 10^{-6} \text{ K}^{-1}$ between 20 and 727 °C, and Al_3Fe with an average CTE of $14.9 \times 10^{-6} \text{ K}^{-1}$ between 20 and 577 °C. Furthermore, the CTE of $(\text{Al}_{0.89}\text{Cr}_{0.11})_3\text{Ti}$ (Al–8Cr–25Ti) was reported as $15.6 \times 10^{-6} \text{ K}^{-1}$ between 20 and 1000 °C [12]. All values are within the range of $(16 \pm 1) \times 10^{-6} \text{ K}^{-1}$ measured for Al_3Sc . We note that Al_3U , $(\text{Al}_{0.89}\text{Cr}_{0.11})_3\text{Ti}$ and Al_3Sc share the same L_{12} 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 Al_3Nb , which has a different DO_{22} structure and a much higher melting point of 1680 °C, was reported as $9.6 \times 10^{-6} \text{ K}^{-1}$ between 20 and 1000 °C [13].

For high-temperature structural use of aluminum alloys strengthened with nano-size, coherent $\text{Al}_3(\text{Sc},\text{X})$ 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 $\text{Al}_3(\text{Sc},\text{X})$ precipitates and the matrix, for which the present measurements of CTE are useful.

The mismatch in lattice parameter between Al and Al_3Sc 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 Al_3Sc , respectively [10,14]. Given the larger CTE and smaller lattice constant of Al as compared to Al_3Sc , the mismatch decreases with increasing temperature. The lattice mismatch between Al and the binary and ternary Al_3Sc phases studied here is plotted in Fig. 3 between

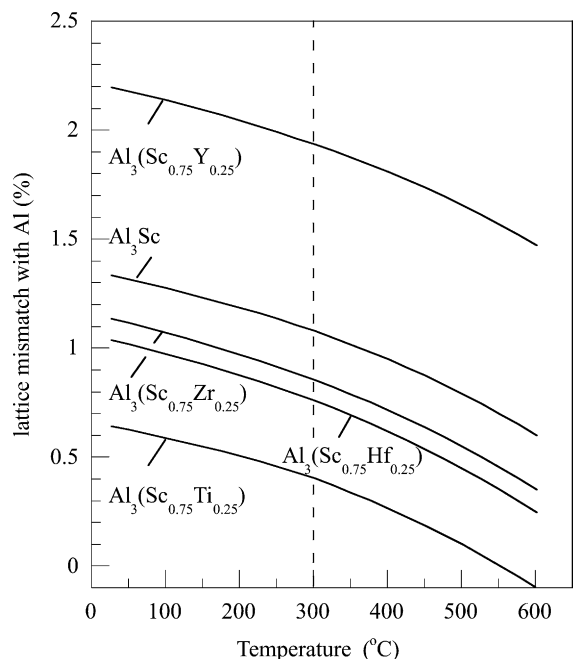


Fig. 3. Calculated lattice mismatch between Al and Al_3Sc or $\text{Al}_3(\text{Sc}_{0.75}\text{X}_{0.25})$ as a function of temperature.

25 and 600 °C, using the temperature-dependent CTE of Al [11], the average CTE values from Fig. 2 for Al_3Sc and $\text{Al}_3(\text{Sc}_{0.75}\text{X}_{0.25})$, 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 $\text{Al}_3(\text{Sc}_{0.75}\text{Ti}_{0.25})$ more than halves the lattice mismatch at 300 °C, as compared to Al_3Sc (Fig. 3). On the other hand, Y additions can increase the mismatch by, e.g., almost a factor 2 for $\text{Al}_3(\text{Sc}_{0.75}\text{Y}_{0.25})$ 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_3Sc and ternary $\text{Al}_3(\text{Sc}_{0.75}\text{X}_{0.25})$, where X is Ti, Y, Zr or Hf, was measured by dilatometry as $(16 \pm 1) \times 10^{-6} \text{ K}^{-1}$. This value is constant between 25 and 900 °C and insensitive to alloying additions. Good agreement is found with a literature value of $14 \times 10^{-6} \text{ K}^{-1}$ calculated from first principles for Al_3Sc , and with published CTE values for other L_{12} tri-aluminides. CTE values for Al_3Sc and $\text{Al}_3(\text{Sc}_{0.75}\text{X}_{0.25})$ 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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