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A Subnanoscale Study of Mg Segregation at Al/Al_3Sc Interfaces

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Three-dimensional atom-probe (3DAP) microscopy provides quantitative chemical information concerning an analyzed specimen on an atomic scale, and is complementary to high-resolution electron microscopy (HREM) for the study of complex precipitation processes in aluminum alloys [1]. This paper presents a specific aspect of the precipitation behavior in Al-Mg-Sc alloys, with experimental measurements of Mg segregation at coherent Al/Al_3Sc interfaces using 3DAP microscopy.

A cast Al-2 wt.% Mg-0.2 wt.% Sc alloy was annealed at 618°C in air for 24 hours, quenched into cold water, and then aged in air at 300°C for times between 0.5 and 1040 hours. 3DAP microscopy tips with an end radius less than 80 nm were obtained by a double electro-polishing technique. Field evaporation was performed at 30 K with a pulse fraction of 20 % at a frequency of 1500 Hz. Between five and 12 Al_3Sc precipitates were analyzed for each aging treatment.

Al_3Sc precipitates are formed with a high number density (about 10^{22} precipitates m^{-3}), which is required for 3DAP microscope observations. The Sc concentration in the matrix decreases with aging time, as expected due to the growth of the Al_3Sc precipitates. The average precipitate radius increases with aging time, in agreement with measurements by HREM. The composition of the Al_3Sc precipitates is 27±1.4 at.%, which is close to the stoichiometric composition. The Al_3Sc precipitate shown in Fig. 1a is defined using an isoconcentation surface corresponding to a composition threshold of 18 at.% Sc [2]. This particular data set was obtained by collecting the evaporating ions near a 110 pole, and Fig. 1b demonstrates the atomic resolution of atom-probe microscopy: every other (110) plane contains Sc atoms, in agreement with the $L1_2$ structure of the Al_3Sc precipitates. The proximity histogram of the same precipitate clearly exhibits an enhanced Mg concentration by a factor of 3 at the Al/Al_3Sc interface (Fig. 2). This segregation behavior is observed for all heat-treatments studied and a quantitative measure is given by the relative Gibbsian interfacial excess of Mg with respect to Al (Γ^{Al}_{Mg}), which is independent of the locus of the dividing surface. It is defined as [3]:

$$\Gamma^{Al}_{Mg} = \Gamma_{Mg} - \Gamma_{Al}\frac{c^{\alpha}_{Mg} - c^{\beta}_{Mg}}{c^{\alpha}_{Al} - c^{\beta}_{Al}}$$

where Γ_{Mg} and Γ_{Al} are the Gibbsian interfacial excesses of Mg and Al, and the c^i_j are the concentrations of component j (j = Al or Mg) in phase i (i = Al or Al_3Sc). The measured value is 2.7±1 atom nm^{-2} for all heat-treatments, demonstrating that the system is in global equilibrium; i.e., the root-mean squared diffusion distance for Mg is much greater than the inter-precipitate spacing.

This study provides direct experimental evidence for first-principles calculations by Asta et al., who showed that Mg should segregate at Al/Al_3Sc (100} interfaces [4]. It also explains morphological changes of Al_3Sc precipitates, e.g. disappearance of faceting for the {100} and {110} planes. Future work will involve discussion of the driving force for Mg segregation at the coherent interface, i.e. elastic strain relaxation or electronic effects.

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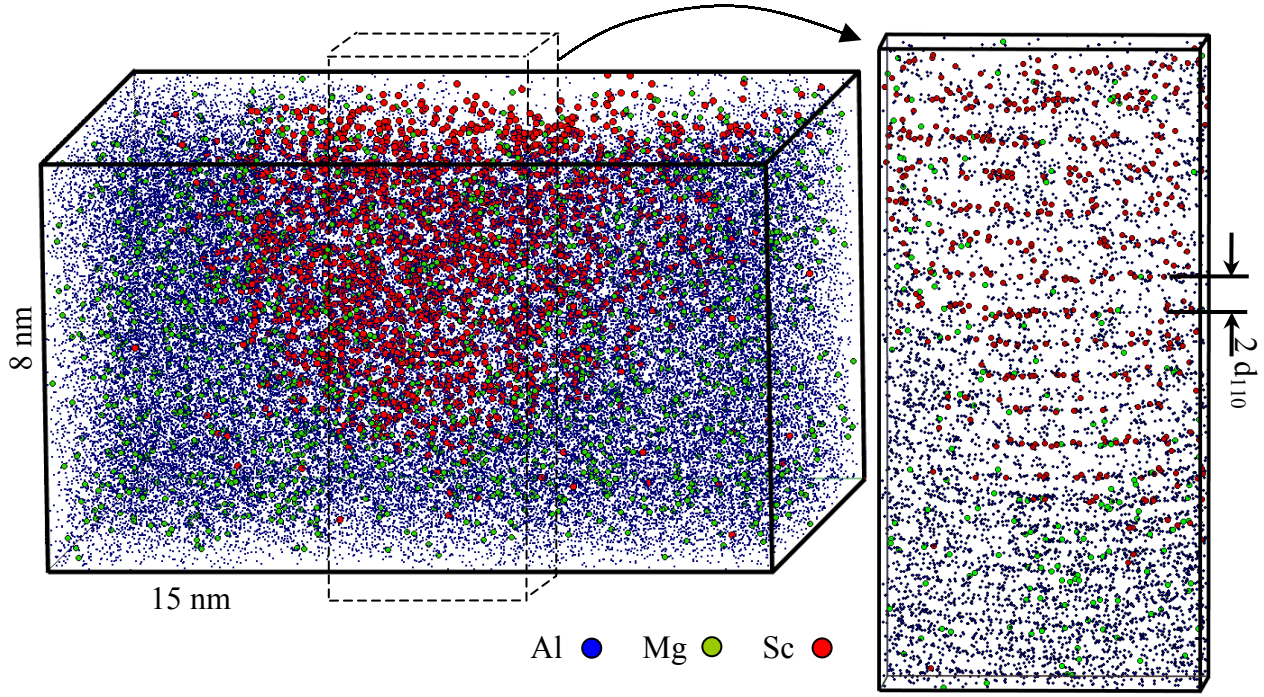

Fig. 1: (a) 3D reconstruction of an Al_3Sc precipitate analysed after aging at 300°C for 1040 hours (b) Slice showing the [110] planes.

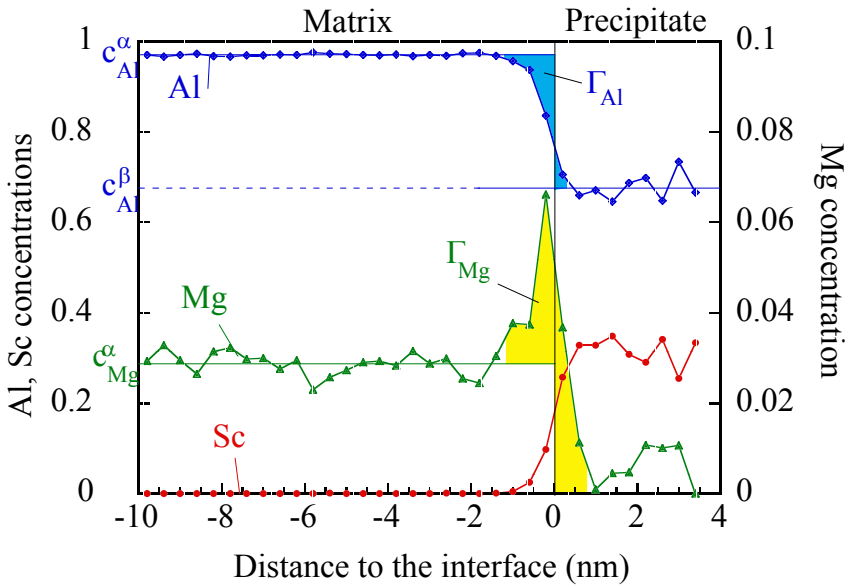

Fig. 2: Proximity histogram for a Al_3Sc precipitate obtained after aging at 300°C for 1040 hours.