Chemical and Structural Investigation of Internal Domains of Needle-Like Ti$_3$AlC Carbide Precipitates in γ-TiAl with 3-D Atom Probe Tomography

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Titanium aluminide (TiAl) alloys have shown improvements in high temperature creep resistance, due in large part to the addition of carbides in the microstructure. Two types of carbide precipitates increase the creep resistance: Ti$_2$AlC [1] and Ti$_3$AlC [2]. There is evidence, however, that hexagonal Ti$_2$AlC carbides (H type) are formed from the metastable perovskite Ti$_3$AlC carbides (P type). Therefore, the nucleation and growth of Ti$_3$AlC precipitates is of interest due to their subsequent transformation into the Ti$_2$AlC phase, which is a stable phase above 800ºC.

Domains within the needle-like carbide precipitates have been observed via strain-field contrast in transmission electron microscopy (TEM), Fig. 1, and high-resolution TEM, Fig. 2. The latter provides evidence that structurally coherent atomic columns traverse the domain boundaries. The chemical makeup of these domains has not been previously investigated. In the current work, three dimensional atom probe (3DAP) microscopy is utilized for resolving the chemical nature of these boundaries [3]. Applying one-dimensional analysis cylinders along the primary axis of P type carbides in 3D reconstructions, Fig. 3, makes possible the measurement of the chemical composition variations inside the carbide precipitates. The nominal composition of the γ-TiAl alloy is Ti$_{50}$Al$_{48}$CMo, with C added for carbide formation and Mo providing increased ductility [4].

After 24 hrs. at 800ºC (Fig. 4a) the domains have a mean composition of Ti$_{67}$Al$_{21}$C$_{11}$O$_1$Mo$_{0.4}$. At the domain boundaries, the Ti, Al, and Mo concentrations are ca. 57, 30, and 2.5 at.%, respectively. After 48 hrs. at 800ºC (Fig. 4b), the domains have a mean composition of Ti$_{67}$Al$_{20}$C$_{11}$O$_{1.3}$Mo$_{0.7}$, and the composition fluctuations at the domain boundaries are less well defined, particularly in the case of the Mo concentration profile, and are indistinguishable from the average domain concentration. The alteration of domain boundary chemical composition reveals the initial steps in the transformation from a P-type to an H-type carbide.

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Fig. 1. TEM micrograph showing P-type carbide precipitates. The beam is oriented along TiAl[310].

Fig. 2. HREM micrograph displaying periodic domain structures and their coherency with the matrix.

Fig. 3. A 15x15x22 nm$^3$ 3DAP microscope reconstruction. The precipitate is defined by a 5 at.% C isoconcentration surface and atoms are shown as Al:red, Ti:green, Mo:blue and C:black.

Fig. 4. Concentration profiles along the axes of P-type carbide precipitates. (a) alloy heat treated at 800°C for 24 hrs., arrows show periodic localized concentration variations. (b) alloy heat treated at 800°C for 48 hrs. where similar concentration variations are observed (except in Mo); the transition to the matrix phase through the end of the precipitate is also shown.