Predicting the early stages of solid-state precipitation in Al-Pt alloys

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Precipitation hardening is an important strengthening mechanism in structural Aluminium (Al) alloys. Among these alloys, the Al-Cu system is a classic, textbook alloy system to investigate the mechanisms of precipitation. In Al-Cu alloys, this strengthening is mainly driven by θ’ (Al2Cu) phase [1]. It has a plate-like shape with high aspect ratios, hence can constitute effective barriers to the movement of dislocations. Given the important role θ’ plays in strengthening Al-Cu alloys, it is important to examine if other θ’-like precipitates exist in Al alloys and what their precipitation characteristics are. This knowledge is likely to be crucial for further development of high strength Al alloys.

Using a combination of systematic density-functional theory (DFT) and classical nucleation theory (CNT) calculations, we design a straightforward workflow to predict the solid-state precipitation in the relatively unexplored Al-Pt alloy system (see Fig.1) [2]. This alloy system is chosen because it contains a simple intermetallic phase, Al2Pt, which is structurally similar to the θ’ phase [3]. This workflow can be applied to an arbitrary binary alloy system. Applying this workflow on the Al-Pt binary system, we calculate the thermodynamics of reported intermetallic phases, and reveal the possible existence of two phase of chemical formulae Al5Pt and Al3Pt. We find this large number of intermetallic phases is due to the strong bonding between Al and Pt, which also leads to significant favourable Pt solute formation energy in the Al matrix. Our findings are compared with the known precipitation characteristics of the binary Al-Cu and Al-Au system. We find that the θ’-like Al2Pt precipitate phase has a lower coherent interfacial energy than θ’. Our calculations strongly suggest that Al2Pt will precipitate first in Al-rich Al-Pt alloys and will form bulk-like interfaces similar to η (Al2Au) [4] rather than like θ’ (Al2Cu) [5].

Figure 1. A workflow to predict the solid-state precipitation in the Al-Pt binary alloy system. Input parameters for CNT are calculated based on DFT. The Al2Pt phase will precipitate first according to our CNT calculations.

Our characterisation of Al-Pt binary system reveals a potential approach for studying solid-state precipitation and discovering high-performance Al alloys. Meanwhile, the proposed workflow can be used in an arbitrary alloy system, which may motivate experimental works in unexplored Al alloy systems.