Designing new alloys for the next generation of jet engines

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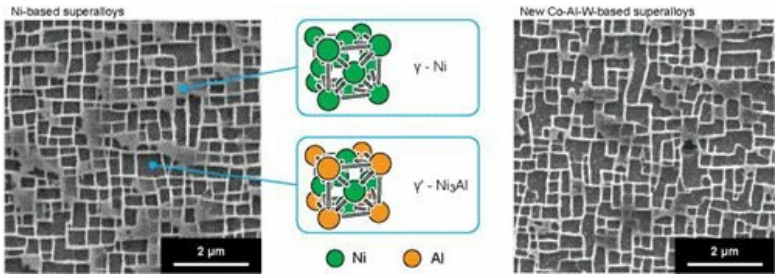
I am a metallurgist. The word metallurgy usually sparks thoughts of loud hot workshops, filled with furnaces and forging presses, where people bash metals. The truth is, I never bash metal and I seldom go to a laboratory. My work focuses on computer modelling to try to understand why alloys (mixes of metals) behave the way they do. Over the years, I have discovered that metals and alloys can still surprise us with new and interesting properties and behaviour. The development of new advanced alloys is indeed a lively and active research area.

Advanced metal alloys have traditionally been designed via time-consuming and expensive trial-and-error approaches. For example, single-crystal, nickel-based (Ni-based) superalloys, used in the hottest stages of jet engines, have taken 60 years of development to get to where they are today. Nowadays, these alloys can withstand many hours of service while exposed to gas temperatures above their melting point. This is possible, in part, thanks to engineering solutions: cooling channels and thermal barrier coatings. The structural material itself, however, also needs to remain strong in these conditions. This is achieved by fine tuning the 10-element-strong composition and perfecting the manufacturing route. The reason why alloys resistant to a higher temperature are desirable is simple—higher temperatures result in increased fuel efficiency. By some estimates, a 30°C increase in operating temperature corresponds to a 1% increase in engine efficiency, and can lead to £12 m in fuel savings over the lifetime of a single large gas turbine.

The quest for a new superalloy

Unfortunately, after decades of continuous development, Ni-based superalloys are currently at their upper operating temperature limit. A suitable alloy system to replace Ni-based superalloys should be identified, but finding this alternative alloy system is not easy. These superalloys owe their exceptional properties to a two-phase system: γ, the native phase of pure Ni, and γ', which is the phase of the compound Ni3Al (see picture). The γ' phase is actually very similar to the γ phase, except that the Ni and Al atoms are arranged in a strict order, avoiding Al-Al nearest neighbour bonds. The special properties of these two phases lead to the formation of a microstructure consisting of little hard γ' phase cubic-shaped precipitates (the bricks) embedded in a matrix of γ phase (the mortar), as shown in the picture. This ‘bricks and mortar’ microstructure is exactly what you need to form a material fine-tuned for strength at high temperatures.

In order to find a new system to replace conventional Ni-based superalloys, we need this bricks and mortar microstructure. Initially, it appeared that the only binary system possessing the necessary combination of phases was the Ni-Al system, upon which conventional superalloys are based. In 2006, however, the γ/γ' microstructure was discovered in the Co-Al-W system (see picture). Replacing Ni-based superalloys with Co-Al-W-based superalloys appears promising: the melting temperature of these new alloys is 100°C higher than current commercial Ni-based superalloys. Will this result in alloys capable of working at 100°C higher than what is possible today? Much work is still needed in order to confirm this. First, the Co-Al-W-based superalloys’ composition should be tweaked to promote the presence of the γ' phase at higher temperatures (you would not want the bricks of your house to disappear). Second, the γ phase should be made more resistant to deformation (you would not want the mortar of your house to crumble away).



Pioneering design and modelling methods

These two objectives can probably be achieved by adding other chemical elements and modifying composition of the Co-Al-W-based superalloys. Yet it is unfeasible to attempt this via trial-and-error experimental means: it took 60 years to perfect Ni-based superalloys, but such abundance of time is now a luxury. This is where state-of-the-art alloy design and modelling methods get to play an important role. My research revolves around using first-principles modelling methods, based on the density functional theory (DFT), to aid the alloy design process. That is, predicting the behaviour of atoms without input from experiments.

The prospect of using first-principles modelling methods to design the new Co-Al-W-based superalloys is extremely exciting. In the School of Metallurgy and Materials, part of my research focuses on the γ' phase in new and conventional superalloys and on how certain solute additions make the γ' phase more resistant to high-temperature deformation. This work will accelerate the introduction of new classes of superalloys to a new generation of jet engines and gas turbines, capable of much higher fuel efficiencies.

Being a Fellow

Being a Birmingham Fellow will allow me freely to follow and implement my own research plans over the next five years. One of the attractive features of the University is its links to many industries focussing on advanced alloys systems. This, will allow me maintain a fruitful two-way knowledge transfer activity with relevant industrial partners. It is where I want to be: using fundamental theory and knowledge to help develop new advanced alloy systems for the benefit of industry and society.