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Alloy development from first principles

Case study

Client Profile
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Product Used
Ni-based superalloys

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Challenges

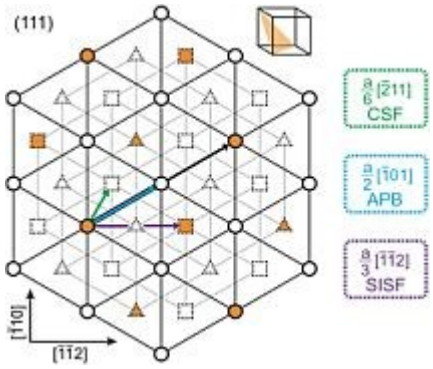
Advanced alloys such as Ni-based superalloys and Ti-alloys are traditionally developed through bucket-chemistry approaches. New compositions are tried, tested and modified, and the process is repeated many times. This approach is slow and expensive. In addition, design criteria rapidly change often due to conditions outside of our control. For example, improvements in single-crystal Ni-based superalloys in the past 20 years have largely been due to the addition of small amounts of Re to the alloy composition. Recently, however, manufacturers are looking to reduce the level of Re in these alloys due to costs and strategic considerations. We therefore must develop faster alloy development approaches that are based on fundamental scientific principles.

Background

The performance of advanced alloys under a variety of conditions is strongly dependent on their composition. The compositions are selected to produce alloys with the desired phases in the optimal quantities. More recently, compositions are tweaked to modify the properties of individual phases. The aim is to optimise the composition to exploit a wide range of atomic-scale phenomena that lead to superior properties. Many of these atomic-scale phenomena can be assessed and studied with atomic-scale electronic-structure simulations, such as those made using density functional theory.

Results

Our research currently focuses on understanding the effect of alloy composition on diffusion properties and deformation mechanism. We use density functional theory to simulate how atoms diffuse in various structures, in order to understand how composition may be used to promote or hinder some of these diffusion mechanisms. We also use density functional theory to simulate how atoms affect planar fault energies, which in turn control many deformation mechanisms in advanced structures. Some of our results have shed light on how certain atoms may have mixed and unexpected diffusion behaviour, and how the whole composition of a phase must be considered when assessing planar fault energies.



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