Optimization of Ni-based superalloys

Calculating interface energy of Ni-based superalloys using density functional theory

***B. N. Ngo-Dinh, M. Bäker, J. Rösler**, Institut für Werkstoffe, Technische Universität Braunschweig*

In Short

- Calculating interface energy of Ni-based superalloy using density functional theory.
- Studying the influence of interface stacking sequence on interface energy
- Studying the influence of alloying elements on interface energy
- Studying the influence of magnetic effects on interface energy

Due to its outstanding mechanical behavior at high temperature, Ni-based superalloys 718 are widely used in production of heavily loaded components of turbines. The excellent strength of these alloys is due to interactions between several phases, either during production or at service. Understanding the interfacial properties of the interface between these phases is thus crucial for designing and optimizing the alloy. Here, we are particularly interested in three interfaces: γ/γ'', γ/δ, and γ/η.

The γ'' phase precipitates as disc-shaped particles in the γ matrix. Due to the orientation relationships $(001)_{\gamma''} \parallel \{001\}_{\gamma}$ and $[100]_{\gamma''} \parallel \langle 100\rangle_{\gamma}$, there are two possible coherent interfaces which are parallel to the $(001)_{\gamma''}$ and $(100)_{\gamma''}$ surfaces, respectively. These particles however coarsen at elevated temperatures during hot working. Moreover, during forging, the fine grains of the alloy grow. Such grain growth can be prevented by precipitating δ and η phases. Knowledge of the respective interface energy proves to be crucial in understanding the ongoing process.

In this project, we will investigate the interface energy of these interfaces, using density functional theory. This work is based on the preceeding works [1–3], in which the stability of particular phases and, to some extent, the interface energy of δ and η were investigated.

Our initial results put the interface energy of two possible coherent γ/γ'' interfaces in the order of about $30 - 50\,\mathrm{mJ/m^2}$. Their interface stress suggests that while the γ''_{001} interface is under compression, the γ''_{100} interface is in tension.These results will provide a precursor for subsequent studies on the interfacial properties of γ/γ'' interface in this project.

There are several possible stacking sequences at the γ/δ and γ/η interfaces. For example, because the stacking sequences of γ-phase and δ-phase are ABCABC and ABAB, respectively, the stacking sequence at the interface can be ABC|AB, ACB|AB, BAC|AB, and CAB|AB. Preliminary calculations show that the difference between interface energy of interfaces with different stacking sequence can be as large as 60 mJ/m^2. In this project, we will investigate the variation of δ and η interface energy with respect to the stacking sequence by calculating the interface energy for all possible stacking sequences. Moreover, we will assess the influence of various relevant alloying elements positioning either in the bulk or at the interface.

Previous study on γ/δ and γ/η interfaces [1] has shown that various alloying elements (Cr in δ-phase, and Mo, W in η-phase) will lower the interface energy and would thus retard particle growth during forging. Following a similar path, we will study the influence of relevant alloying elements on the interface energy of the γ/γ'' interface.

In their study, Woodward et al. [4] pointed out that magnetic effects strongly influence the interface properties of γ/γ' interface. Our initial calculation has also shown that turning off the magnetic effect might even invert the sign of the interface energy. This comes from the fact that, for example, while pure Ni is ferromagnetic, bulk δ phase is nonmagnetic. We will dedicate the last past of the project on assessing the influence of magnetic effects on the interface energy by using non-spin-polarized calculations.

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More Information

[1] Bäker, Martin; Rösler, Joachim, Effects of alloying on the interface energy of the δ-and η-phase in nickelbase superalloys. *Modelling and Simulation in Materials Science and Engineering* 27 (1) pp. 015002. doi:10.1088/1361-651X/aaefc1

[2] Bäker, Martin; Rösler, Joachim; Hentrich, Tatiana;Ackland, Graeme, Influence of transition group elements on the stability of the δ-and η-phase in nickelbase alloys. *Modelling and*

Simulation in Materials Science and Engineering 26 (1) pp. 015005. doi:10.1088/1361-651X/aa9759

[3] Bäker, Martin; Rösler, Joachim, Influence of transition group elements on the stability of the γ"-phase in nickelbase alloys. *Modelling and Simulation in Materials Science and Engineering*. doi:10.1088/1361-651X/abd043

[4] Woodward, C; Van De Walle, Axel; Asta, Mark; Trinkle, DR, First-principles study of interfacial boundaries in Ni–Ni_3Al. *Acta materialia* 75 pp. 60–70. doi:10.1016/j.actamat.2014.04.056

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