Interfaces in Ni-base superalloys and implications for mechanical behavior and environmental embrittlement: a first-principles study

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Abstract
Motivated by the vital role played by grain boundaries and interfaces in Ni-based superalloys in influencing mechanical properties such as creep rupture strength, fatigue crack growth rates and resistance towards environmental embrittlement, we use first-principles simulations to estimate fracture strengths of Ni interfaces in Ni-base superalloys in different proportions, depending on alloying, processing and heat-treatment conditions. These interfaces and grain boundaries have been found to play a critical role in controlling the bulk mechanical properties of these alloys [2]. Hence, to gain a more complete understanding of the mechanical responses of these alloys in terms of resistance to crack propagation through interfaces/grain boundaries, it is insightful to compare the fracture strengths of the various interfaces/grain boundaries.

Introduction
In multi-element Ni-base superalloys used in high-temperature applications such as turbine disks, microstructures consist of multiple phases, such as γ', γ, carbides, borides [1]. Complex interfaces, including γ/γ, γ/γ' interfaces and γ/Boride interfaces coexist in Ni-based superalloys in different proportions, depending on alloying, processing and heat-treatment conditions. These interfaces and grain boundaries have been found to play a critical role in controlling the bulk mechanical properties of these alloys [2]. Hence, to gain a more complete understanding of the mechanical responses of these alloys in terms of resistance to crack propagation through interfaces/grain boundaries, it is insightful to compare the fracture strengths of the various interfaces/grain boundaries.

Under certain combinations of stress and temperature, many materials will tend to fail in an intergranular fashion [3]. A proposed solution to this problem has been to percolate the microstructure with boundaries having an increased resistance to fracture, via appropriate processing routes [4]. A simplified way to characterize a grain boundary between two grains involves the coincidence-site-lattice (CSL) model, in which the relative orientation of the two grains is given by a ΣN value, where one out of N atoms along the grain boundary is coincident [5]. Hanada et al [6] and Lin et al [7] have established that in Ni3Al, low-angle and Σ3 symmetrical boundaries are especially resistant to cracking and therefore are considered as “strong boundaries”. J. Q. Su et al [8] furthered this study by establishing that while Σ1, Σ3, and Σ9 boundaries in Ni3Al are crack-resistant, Σ3, Σ7, Σ11, Σ13 and random boundaries are weaker, fracturing preferentially to the bulk intragranular material. These studies qualitatively establish a relationship between fracture properties and the type of grain boundary based on its Σ-value. However, to the best of our knowledge, there has been no modeling study around prediction of fracture strengths and their correlation with grain boundary character distribution.

The susceptibility of Ni-based superalloys as well as Ni-Ni3Al based alloys to environmental embrittlement is well documented [9-10]. Ni-based superalloys can experience accelerated crack growth rates under the combined effects of environment, stress, and temperature [1, 11-14]. Careful experiments done on air-exposed Ni270 (99.98 pct Ni) specimens exhibit large regions of intergranular failure, contrasted with their vacuum-exposed counterparts which show ductile behavior [14].

Addition of boron is reported to be beneficial in reducing environmental embrittlement in various Ni-based superalloys [15-16]. B atoms are found to segregate to grain boundaries and bind to grain boundary sites, or precipitate as boride particles along grain boundaries in Ni-base superalloys [17]. Considering the potential impact of borides at grain boundaries on mechanical responses of Ni-based alloys [17-19], an understanding of the fracture strengths of boride-containing interfaces has become critical.

Experimentally, a sample always contains different types of grain boundaries and interfaces and it is hard to study their relative strengths and role in determining fracture behavior or embrittlement. Over the last decade, there has been a significant amount of theoretical work developing relationships between specific Ni-based superalloy interfaces and their bulk mechanical properties. For example, sulfur-induced embrittlement of Ni has been studied by Yamaguchi et al [20] through first-principles calculation of grain boundary decohesion in Ni-Σ2(012). However, the fracture strength of Ni grain boundaries as a function of environmental effects and grain boundary character distribution has not been studied in details. The next predominant interface in Ni-base superalloys is the γ/γ' interface as a typical microstructure contains ~50% of its volume fraction as γ' precipitates. The γ/γ' interface has been widely studied using first-principles quantum mechanical calculations to investigate the strengthening mechanisms of a variety of alloying metal
environmental embrittlement on select interfaces using first-principles density functional calculations. Tilt boundaries and 

1(a)). Following a similar procedure, the crystal was then reflected in the surface plane. The two grains and details of creation of the grain boundaries/interfaces and is described in Section 2. Discussions are provided in Section 3. Our findings are summarized in Section 4.

This paper is organized as follows. The methodology including a description of the first-principles based computational technique and methods of creation of the grain boundaries/interfaces and is described in Section 2. Discussions are provided in Section 3. Our findings are summarized in Section 4.

**Methodology**

**Computational Details**

We use first-principles Density Functional Theory [28-29], as implemented in the Vienna Ab initio Simulation Package (VASP) [30], with the Perdew-Wang [31] function of the Generalized Gradient Approximation (GGA) to exchange-correlation energy, with no dependence on electronic spin. Projector-augmented wave potentials [32] are used to describe the computationally expensive electron-ion interactions, which permitted the use of a plane-wave basis set with energy cutoff of 400 eV in the representation of the Kohn-Sham wave functions. The Brillouin Zone integrations are sampled with a 3x3x2 Monkhorst-Pack grid [33] in a calculation consisting of 8 atomic planes of Cr5B3 and 4 atomic planes of (001)orientation relationship of the γll (001)M5B3, the Ni/Cr5B3 interface has been constructed, with a BCT structure and lattice parameters of a = 5.4 Å, c = 10.1 Å, and c/a = 1.83. They have carried out compositional analysis by x-ray spectroscopy in the transmission electron microscope to establish that the primary constituents of these borides are Cr, Mo & W. Structural optimization of bulk relaxations of I4/mcm Cr5B3 yielded lattice constants aCr5B3 = 5.37 Å and cCr5B3 = 10.18 Å which are in excellent agreement with the experimental values of aCr5B3 = 5.4 Å, cCr5B3 = 10.1 Å, respectively. Based on these bulk configurations and the orientation relationships of boride precipitates with γ-grain boundaries. Zhang et al [36-37] have carried out extensive characterization of IN738 and Rene 80 to establish the boride precipitates along γ-grain boundaries to be Cr7B2-type M23B6, with a BCT structure and lattice parameters of a = 5.4 Å, c = 10.1 Å, and c/a = 1.83. They have carried out compositional analysis by x-ray spectroscopy in the transmission electron microscope to establish that the primary constituents of these borides are Cr, Mo & W. Structural optimization of bulk relaxations of I4/mcm Cr5B3 yielded lattice constants aCr5B3 = 5.37 Å and cCr5B3 = 10.18 Å which are in excellent agreement with the experimental values of aCr5B3 = 5.4 Å, cCr5B3 = 10.1 Å, respectively. Based on these bulk configurations and the orientation relationships of the γ/Boride interface being variants of (001), (011), or (001), the Ni/Cr5B3 interface has been constructed, consisting of 8 atomic planes of Cr5B3 and 4 atomic planes of FCC Ni, i.e., 52 atoms (Fig. 1(d)). This semi-coherent interface has a lattice constant of a = 5.46 Å with a lattice mismatch of 1.1% with Cr5B3. The effect of boride chemistry on interfacial strength is studied through a 50% Mo-for-Cr substitution within the Cr5B3 boride (Fig. 1(e)), see ref. [27] for details.

Finally, the γ/Boride interface is created based on reported experimental data on the orientation relationships of boride precipitates with γ-grain boundaries. Zhang et al [36-37] have carried out extensive characterization of IN738 and Rene 80 to establish the boride precipitates along γ-grain boundaries to be Cr7B2-type M23B6, with a BCT structure and lattice parameters of a = 5.4 Å, c = 10.1 Å, and c/a = 1.83. They have carried out compositional analysis by x-ray spectroscopy in the transmission electron microscope to establish that the primary constituents of these borides are Cr, Mo & W. Structural optimization of bulk relaxations of I4/mcm Cr5B3 yielded lattice constants aCr5B3 = 5.37 Å and cCr5B3 = 10.18 Å which are in excellent agreement with the experimental values of aCr5B3 = 5.4 Å, cCr5B3 = 10.1 Å, respectively. Based on these bulk configurations and the orientation relationships of the γ/Boride interface being variants of (001), (011), or (001), the Ni/Cr5B3 interface has been constructed, consisting of 8 atomic planes of Cr5B3 and 4 atomic planes of FCC Ni, i.e., 52 atoms (Fig. 1(d)). This semi-coherent interface has a lattice constant of a = 5.46 Å with a lattice mismatch of 1.1% with Cr5B3. The effect of boride chemistry on interfacial strength is studied through a 50% Mo-for-Cr substitution within the Cr5B3 boride (Fig. 1(e)), see ref. [27] for details.

The fracture strength of an interface between grains X and Y is assessed through determination of the cleavage energy, $\gamma_{cl}$. $\gamma_{cl}$ is essentially the work of separation [38] and defined as

$$\gamma_{cl}^{XY} = \gamma_{X}^{Y} + \gamma_{Y}^{X} - \frac{E_{int}}{2A}$$

For example, for an interface between Ni and Boride, cleavage energy is given by $\gamma_{cl}^{Ni/boride}$, where,
A comparison of cleavage energies across Ni/Cr5B3 interfaces, Ni/Cr5B3 and Ni/Cr2.5Mo2.5B3 interfaces (5.15 & 5.08 J/m², grain boundaries reveals notable trends. The cleavage energy of crystallographic orientations of the same material. The details of a grain boundary, X and Y correspond to different symmetric tilt boundaries are stronger than the boundary, Σ3(111) symmetric tilt boundaries need higher energies to cleave over Ni. Suzuki et al [39] experimentally determined the fracture strengths of different CSL grain boundaries in Ni-20Cr using a microtensile test method to show the fracture strength of Σ3(111) grain boundaries are higher than that of Σ5(012) boundaries. Our finding is also consistent with experimental measurements of grain boundary fracture strengths done on FCC intermetallic compound Ni3Al where Su et al [8] report the fracture strengths of Σ3 grain boundaries to be higher than that of Σ5.

A comparison of cleavage energies across Ni/Cr5B3 interfaces, Ni/Ni3Al interfaces, Ni/Σ5(012) grain boundaries and Ni/Σ3(111) grain boundaries reveals notable trends. The cleavage energy of Ni/Cr5B3 and Ni/Cr5B3/Mo2B3 interfaces (5.15 & 5.08 J/m², respectively) is found to be higher than those obtained for the Ni/Ni3Al interface (4.22 J/m²) and Ni grain boundaries (3.60 & 3.81 J/m²). This indicates that fracture strengths of the Ni/Boride interfaces are intrinsically higher than that of NiΣ5 & Σ3 grain boundaries and coherent Ni/Ni3Al interfaces in Ni-base alloys. This finding is consistent with experimental observations that addition of B increases the creep rupture strength and decreases the fatigue-crack-growth rates in Ni-base superalloys [15, 18]. Rosler et al [15] demonstrated significant life extension in INCONEL 706 by chemical modification of a surface zone with B and established that the B was present as boride precipitates in the matrix zone. Xiao et al [18] reported that addition of B improved the crack growth resistance of IN 718 at room temperature and at 650°C. With increasing B concentration, the fracture mode in these alloys was found to change from intergranular- to transgranular, indicating a change in interfacial cohesion.

It is interesting to compare our current findings with earlier calculations, where we had placed B as an interstitial dopant along a Ni-Σ5(012) grain boundary, at a concentration of 2.4 atomic% [30]. The cleavage energy of Ni-Σ5(012) grain boundary with atomic B (3.82 J/m²) was found to be higher than that of a undoped grain boundary (3.60 J/m²), thereby establishing that even during equilibrium segregation of B at grain boundaries, B acts as a strengthener. During non-equilibrium segregation when B is present as boride precipitates along grain boundaries [17], the strengthening effect is found to be even higher, as is evident in the cleavage energy of Ni/Cr5B3 interfaces (5.15 J/m², Figure 2).

### Results and Discussion

#### Comparison of fracture strengths of grain boundaries and interfaces

Calculated cleavage energies for the pure grain boundaries and interfaces are given in Figure 2. A comparison between the two grain boundaries examined in Ni points to the direction that Ni Σ 3(111) symmetric tilt boundaries need higher energies to cleave the boundary over Ni Σ5(012), thereby indicating that Σ3(111) symmetric tilt boundaries are stronger than Σ5(012) in pure Ni. This finding is in accordance with experimental observations. Suzuki et al [39] experimentally determined the fracture strengths of different CSL grain boundaries in Ni-20Cr using a microtensile test method to show the fracture strength of Σ3(111) grain boundaries are higher than that of Σ5(012) boundaries. Our finding is also consistent with experimental measurements of grain boundary fracture strengths done on FCC intermetallic compound Ni3Al where Su et al [8] report the fracture strengths of Σ3 grain boundaries to be higher than that of Σ5.

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#### Effects of oxygen embrittlement

To study the effects of oxygen on interfacial strength, Ni/Ni3Al and Ni/Mo3B3 (M = Cr, Mo) interfaces are chosen.

In the Ni/Ni3Al interface, oxygen segregation is studied by placing one oxygen atom at each of the interfaces, resulting in an impurity concentration of 2.5 atomic%. There are three possible interstitial sites for occupancy by the impurity atoms at the interface, viz. a tetrahedral site constituted by 3 Ni and 1 Al atom; an octahedral site formed by 4 Ni and 2 Al atoms (see Figure 3). The interstitial volumes decrease in the order: Σ5(012) > Σ3(111) > Σ5 & Σ3 grain boundaries.
Despite the above, the most favorable site for O residence is found to be the 4 Ni-2Al octahedral site, followed by the 3Ni -1Al tetrahedral site and the all-Ni octahedral site. Hence the preferred sites at the interstices of Ni/Ni$_3$Al interface for an O dopant seem to be guided more by the chemical interactions than the interstitial space availability. This can be explained by the strong chemical affinity of electronegative O towards Al atoms, which is found to govern its preferences for its nearest neighbors, dictating its interstitial site preferences. The tendency of O to segregate to the $\gamma$/$\gamma'$ interface over residing in the bulk lattice can be determined from the energy difference $\Delta E$, given by:

$$\Delta E = E^{\text{int}}(\text{Ni}_{68}\text{Al}_{12}\text{O}_2) - [E^{\text{bulk}}(\text{Ni}_{32}\text{O}) + E^{\text{bulk}}(\text{Ni}_{36}\text{Al}_{12}\text{O})],$$

where, $E^{\text{int}}(\text{Ni}_{68}\text{Al}_{12}\text{O}_2)$ is the total energy of $\gamma$/$\gamma'$ interface having oxygen at its preferred interstitial site, $E^{\text{bulk}}(\text{Ni}_{32}\text{O})$ is the total energy of oxygen in the preferred interstitial site of bulk FCC Ni, $E^{\text{bulk}}(\text{Ni}_{36}\text{Al}_{12}\text{O})$ is the total energy of oxygen in the preferred interstitial site of bulk L1$_2$ Ni$_3$Al. Our calculations show that O has a strong natural tendency to segregate to the $\gamma$/$\gamma'$ interface (-0.41 eV).

Figure 5. Calculated Cleavage Energies for Ni/Ni$_3$Al and Ni/Cr$_5$B$_3$ (M = Cr, Mo) interfaces, with oxygen.

Cleavage energies for the Ni/Ni$_3$Al & Ni/M$_3$B$_3$ (M = Cr, Mo) interfaces with oxygen at the different preferred sites at the interface are given in Figure 5. A comparison with cleavage energies calculated for undoped Ni/Ni$_3$Al & Ni/M$_3$B$_3$ (M = Cr, Mo) interfaces (Figure 2) show that with introduction of oxygen, there is reduction in cleavage energies in all interfaces, indicating that both Ni/Ni$_3$Al & Ni/M$_3$B$_3$ (M = Cr, Mo) interfaces are weakened. However, the cleavage energy of Ni/Ni$_3$Al interfaces in the presence of oxygen (3.46 J/m$^2$) is lower than that of Ni/boride interfaces in the presence of oxygen (4.27-4.31 J/m$^2$, Figure 5). This suggests that the extent of environmental embrittlement in $\gamma$/boride interfaces is lesser than in $\gamma$/$\gamma'$ interfaces. This result is broadly supported by earlier experimental work on IN706 where O-enhanced-crack-growth rate is lowered by increasing surface concentration of B, which is found to form boride precipitates within the matrix [15].

To assess whether O would spontaneously like to go to a Ni/Ni$_3$Al interface over a Ni/Boride interface, the following energies are estimated:

$$E(\text{Ni/Ni}_3\text{Al}-\text{O}) = E(\text{Ni/Ni}_3\text{Al} + \text{O}) - E(\text{Ni/Ni}_3\text{Al}) - E(\text{O}) \quad (i)$$

$$E(\text{Ni/Cr}_5\text{B}_3-O) = E(\text{Ni/Cr}_5\text{B}_3 + \text{O}) - E(\text{Ni/Cr}_5\text{B}_3) - E(\text{O}) \quad (ii)$$

$$E(\text{Ni/Cr}_{2.5}\text{Mo}_{2.5}\text{B}_3 -\text{O}) = E(\text{Ni/Cr}_{2.5}\text{Mo}_{2.5}\text{B}_3 + \text{O}) - E(\text{Ni/Cr}_{2.5}\text{Mo}_{2.5}\text{B}_3) - E(\text{O}) \quad (iii)$$

Our estimates for these energies are calculated to be -10.58 eV, -6.63 eV and -5.66 eV for (i), (ii) and (iii) respectively. These estimates demonstrate that an O atom prefers to be at the Ni/Ni$_3$Al interface over Ni/Cr$_5$B$_3$ interface by 3.94 eV. Comparison of (i) & (ii) also establishes that O prefers to be at the Ni/Ni$_3$Al interface over Ni/Cr$_{2.5}$Mo$_{2.5}$B$_3$ interface by 4.92 eV. This finding, along with our earlier observation that the effect of O-induced embrittlement is much more severe in Ni/Ni$_3$Al interfaces than in Ni/Cr$_5$B$_3$ interfaces indicates a potential pathway for improving intergranular crack growth resistance in Ni-base superalloys by way of increasing the volume fraction of grain boundary borides.

**Effect of composition of boride on $\gamma$/Boride interfacial fracture strengths**

Based on these calculations, an understanding of the effects of chemistry on the fracture strengths of Ni/Ni$_3$Al & Ni/M$_3$B$_3$ (M = Cr, Mo) interfaces is developed through an examination of the electron localization functions [40] (ELF) (see Figs. 6 & 7). The relative interplay of electronegativities (EN) between the different
atomic species (Ni, Cr, Mo, B, O) is found to hold a key to their interfacial strengths. For pristine Ni/Cr$_5$B$_3$ interfaces in the absence of O, charge transfer across the interface, and hybridization between dissimilar atoms, leads to higher fracture strength than that calculated for a 2Σ(012) Ni grain boundary, Σ3(111) Ni grain boundary or a Ni/Ni$_3$Al interface (see Figure 2). Addition of Mo to the boride reduces the Ni/boride interface strength in the absence of O because of a reduced EN difference between B and Ni. This is a direct consequence of a higher electronegativity of Mo, relative to Cr (EN of Cr = 1.66, EN of Mo = 2.16, EN of Ni = 1.91, EN of B = 2.04, in Pauling Scale).

Oxygen, a strongly electronegative element (EN of O = 3.44, in Pauling Scale) attributing to its embrittlement.

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Strength than that calculated for a hybridization between dissimilar atoms, leads to higher fracture strength in the absence of O because of a reduced EN difference between B and Ni. However, for the interfaces, upon relaxation O atoms approach Cr atoms, the most electronegative atom in the Ni/Cr$_5$B$_3$ interface. This shift in priority demonstrated by the O atom is directly related to the relative electronegativities of its nearest neighbor atoms. This synergistic interplay between different alloying elements present in the interfaces is found to ultimately influence the strength of these interfaces.

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\[ \Sigma \]

Strength in the absence of O because of a reduced EN difference between B and Ni.

In contrast, in the Ni/Cr$_{2.5}$Mo$_{2.5}$B$_3$ interface, the presence of electronegative Mo suppresses the strong electronegative character of O to some extent, resulting in less charge localization around O, which is reflected in the increased strength of the Ni/Cr$_{2.5}$Mo$_{2.5}$B$_3$ interface, relative to its Ni/Cr$_5$B$_3$ counterpart, in the presence of O. The extent of charge localization around O atoms in these two interfaces is evident in the ELF plots (see Fig. 7). It is also interesting to note that although the starting positions of O atoms are kept identical in Ni/Cr$_5$B$_3$ and Ni/Cr$_{2.5}$Mo$_{2.5}$B$_3$ interfaces, upon relaxation O atoms approach Cr atoms, the most electropositive atom in the Ni/Cr$_5$B$_3$ interface. However, for the Ni/Cr$_{2.5}$Mo$_{2.5}$B$_3$ case, where the interface is comprised of Ni, Mo & B atoms with Cr atoms positioned farther from the interface, O is found to move further from Mo, positioning itself at an intermediate position between Ni & B atoms. This shift in priority demonstrated by the O atom is directly related to the relative electronegativities of its nearest neighbor atoms. This synergistic interplay between different alloying elements present in the interfaces is found to ultimately influence the strength of these interfaces.

O is found to induce a strong region of charge concentration around itself when present at an interface (Figs. 6 & 7). It had earlier been established [29-31] that charge localization around a dopant at the interface results in increased ionicity at the interface, thus weakening the interface. A similar region of charge concentration is seen around O in the Ni/Cr$_5$B$_3$ interface (Figure 7) attributing to its embrittlement.

Figure 7. (Color Online) Contour plots of Electron Localization Function in (001) plane for (a) Cr$_5$B$_3$/Ni interface and (b) (Cr,Mo)$_5$B$_3$/Ni interface with oxygen. Extent of charge localization induced by oxygen in the two cases may attribute to the differential strengths of these interfaces. Ref. [27]

Future work in this area would involve exploring different orientation relationships in γ/boride interfaces and also incorporating other variants such as γ′/boride interfaces, to develop a more complete understanding of the effects of boride precipitates in the microstructures of Ni-based superalloys. Keeping in mind the synergistic interplay between different alloying elements and their effects on mechanical responses of interfaces, it would be interesting to extend the current calculations beyond Ni to capture the effect of multi-element γ composition on interfacial strengths.

Our work provides a framework for fundamental understanding of fracture strengths of relevant interfaces in Ni-based superalloys, and should help in identifying alloying additions/processing routes to increase the strengths and proportions of such interfaces. Such approaches would work towards increasing the overall strength of Ni-based superalloys and reducing their environmental sensitivity during service.

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