Quantum-mechanical study of tensorial elastic and high-temperature thermodynamic properties of grain boundary states in superalloy-phase \( \text{Ni}_3\text{Al} \)

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Abstract. Grain boundaries (GBs), the most important defects in solids and their properties are crucial for many materials properties including (in-)stability. Quantum-mechanical methods can reliably compute properties of GBs and we use them to analyze (tensorial) anisotropic elastic properties of interface states associated with GBs in one of the most important intermetallic compounds for industrial applications, \( \text{Ni}_3\text{Al} \). Selecting the \( \Sigma 5(210) \) GBs as a case study because of its significant extra volume, we address the mechanical stability of the GB interface states by checking elasticity-based Born stability criteria. One critically important elastic constant, \( C_{55} \), is found nearly three times smaller at the GB compared with the bulk, contributing thus to the reduction of the mechanical stability of \( \text{Ni}_3\text{Al} \) polycrystals. Next, comparing properties of \( \Sigma 5(210) \) GB state which is fully relaxed with those of a \( \Sigma 5(210) \) GB state when the supercell dimensions are kept equal to those in the bulk we conclude that lateral relaxations have only marginal impact on the studied properties. Having the complete elastic tensor of \( \Sigma 5(210) \) GB states we combine Green’s-function based homogenization techniques and an approximative approach to the Debye model to compare thermodynamic properties of a perfect \( \text{Ni}_3\text{Al} \) bulk and the \( \Sigma 5(210) \) GB states. In particular, significant reduction of the melting temperature (to 79-81% of the bulk value) is predicted for nanometer-size grains.

1. Introduction

Grain boundaries (GBs) are extended defects which are critically important for a number of properties of solid-state materials, including, e.g., their macroscopic strength [1-6]. GBs often possess highly distorted atomic configurations and, therefore, it is advantageous to use reliable theoretical tools, such as quantum-mechanical (so-called first-principles or \textit{ab initio}) calculations, when studying them [7-22]. Their properties are very sensitive to compositional changes [23-36]. GB properties are very sensitive to various (e.g., thermodynamically-driven) compositional changes Also the impurities, even in very low concentrations (ppm), can dramatically change their characteristics (see, for example, Refs. [37, 38]). Intergranular embrittlement, which is
usually associated with segregation of impurities on the GB, is accompanied by a significant reduction of the ductility and strength. Impurities can also drastically reduce local magnetic properties at grain boundaries in magnetic materials, as documented e.g. in elemental Ni (Refs. [39, 40]). In particular, in ultra-fine grained (UFG) or nano-granular materials, GBs can become even more important than the grain interior itself and it is possible to achieve unprecedented properties not available in bulk samples. When reducing the grain sizes to truly nano-scale levels, even elastic properties may become significantly altered by GBs as compared with the bulk.

The principal goal of our research is assess high-temperature thermodynamic properties, in particular the melting temperature, of those material regions which are affected by GBs (the concept of complexion is worth mentioning in this context [41-62]) employing the knowledge of their tensorial elastic properties. Our recent paper [63] as well as the present one thus complement many previous GB-related studies that were focused predominantly on scalar characteristics (energy, strength, changes in inter-atomic bonds) as well as electronic structure and atomic configuration, see e.g. Refs. [24, 64-78]. Tensorial properties require rather computationally demanding approaches (see e.g. [79]) but this disadvantage is compensated by the wealth of insight which is gained. The knowledge of a full elastic tensor allows for assessing the mechanical stability of the studied phases via generic Born stability criteria [80, 81]. Further, elastic properties also play a crucial role in thermodynamic stability as they determine long-wave phonon frequencies and can be employed within classical approximative model of Slater [82] to predict (high-temperature) thermodynamic properties of materials (for example the melting temperature as discussed below).

Here we analyze thermodynamic and tensorial elastic properties of the Σ5(210) grain boundaries in one of the most important intermetallics, Ni₃Al, which appears e.g. as the γ′ phase in Ni-based superalloys. In particular, we study the Σ5(210) GB (see figure 1) which is one of the smallest GBs exhibiting an extra volume (when compared with the bulk), similarly as in many non-special GBs.

2. Methodology

Our \textit{ab initio} calculations were performed within the framework of density functional theory [83, 84] using the Vienna Ab initio Simulation Package (VASP) [85, 86]. The exchange and correlation energy was treated within the generalized gradient approximation as parametrized by Perdew, Burke, and Ernzerhof [87] and implemented in projector augmented wave pseudopotentials [88]. We used a plane-wave energy cut-off of 500 eV with a 5 × 17 × 3 Monkhorst-Pack k-point mesh for the 64-atom supercells, reducing the forces on atoms under 1 meV/Å.

The two different GB chemical compositions corresponding to either both Ni and Al or solely Ni atoms at the GB plane are shown in figures 1a,b. As periodic boundary conditions apply, the supercells are periodic approximants of the real GB-associated interface states. Elastic constants were computed by the stress-strain method outlined in Refs. [89, 90]. For the lower-energy GB variant we compared the results for two different types of simulations (and strain state). First, we determined thermodynamic, structural and tensorial elastic properties when all atomic positions as well as the shape and the volume of the supercell were fully relaxed. Second, we relaxed all the above mentioned degrees of freedom except for the supercell dimensions within the GB plane which we keep equal to the equilibrium values predicted for the bulk Ni₃Al.

Finally, when simulating the application of external strains to determine the elastic constants (see Refs. [89, 90]), we also relaxed the atomic positions. Our tests show that the most critical shear elastic constant, $C_{55}$, that could be as low as 15 GPa in case when only Ni atoms are located at the interface (see more details in our recent paper [63]), is much higher (64 GPa) if these atomic relaxations are omitted.
3. Results

Our recent publication [63] summarizes most of our results related to the elasticity of GB states. The current paper uses these findings to assess high-temperature thermodynamic properties of GB states, in particular differences in the melting temperature when compared to the bulk Ni$_3$Al. A few selected facts from Ref. [63], which are critically important for the thermodynamic modeling discussed below, will be nevertheless briefly discussed here. In particular, our calculations show that the $\Sigma 5(210)^{\text{Al,Ni}}$ with both types of atoms (Al and Ni) at the interface (figure 1a) has a lower GB energy of 1.38 J/m$^2$ (it is 1.66 J/m$^2$ in the case of the $\Sigma 5(210)^{\text{Ni,Ni}}$ with only Ni atoms at the interface - see figure 1b). The lower energy variant $\Sigma 5(210)^{\text{Al,Ni}}$ has the additional volume per unit GB area 0.29 Å$^3$/Å$^2$, i.e. lower than 0.32 Å$^3$/Å$^2$ computed for the higher energy variant $\Sigma 5(210)^{\text{Ni,Ni}}$. Our values related to $\Sigma 5(210)^{\text{Ni,Ni}}$ are in excellent agreement with the previous theoretical results of 1.7 J/m$^2$ and 0.36 Å$^3$/Å$^2$ [8]. Due to the lower energy predicted for the $\Sigma 5(210)^{\text{Al,Ni}}$ variant, we will focus only on this GB state from now on. Calculated elastic constants of $\Sigma 5(210)^{\text{Al,Ni}}$ interface states are given in table 1 together with bulk Ni$_3$Al elastic constants in the same coordination system. The table contains three sets of elastic constants for $\Sigma 5(210)^{\text{Al,Ni}}$ GB states. Two of them are computed for both a fully relaxed state and an interface-constrained state. In the latter case the supercell dimensions within the GB interface are kept constant and equal to the equilibrium values computed for the bulk Ni$_3$Al but the atomic positions, the overall volume, and the supercell size in the direction perpendicular to the GB interface are relaxed so as to minimize the total energy of the studied system. The last set of elastic constants is obtained with the help of a linear-elasticity approach. In order to visualize how the interface states associated with GBs respond to uniaxial loading along different crystallographic directions, we exhibit directional dependencies of the Young’s modulus and linear compressibility in figure 2.
Figure 2. Directional dependencies of the Young’s modulus (a,c,e) and linear compressibilities (b,d,f) computed with the help of quantum-mechanical calculations in case of bulk Ni₃Al (a,b), fully relaxed Σ5(210)\textsuperscript{ALNi} (c,d) and the Σ5(210)\textsuperscript{ALNi} with the supercell dimensions kept equal to those in the bulk (e,f). Please note that the sub-figures (c-f) have their coordination systems defined in figure 1 while those visualizing properties of the bulk Ni₃Al (a,b) have the orthonormal coordination system matching the unit vectors of the elementary cell of Ni₃Al.
Table 1. The \emph{ab initio} computed elastic constants (all in GPa) of (i) the Ni$_3$Al bulk in the coordination system of the studied GBs (shown in figure 1), (ii) Ni$_3$Al $\Sigma 5(210)$ GBs states (see figure 1) both fully relaxed and interface-constrained, and (iii) prediction based on the linear-elasticity approach from Ref. [91].

| Ni$_3$Al states: | $C_{11}$ | $C_{12}$ | $C_{13}$ | $C_{22}$ | $C_{23}$ | $C_{33}$ | $C_{44}$ | $C_{55}$ | $C_{66}$ |
|----------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| bulk $\langle 2\overline{1}0 \rangle \langle 001 \rangle \langle 210 \rangle$ | 298    | 152    | 100    | 246    | 152    | 298    | 128    | 76     | 128    |
| $\Sigma 5(210)^{\text{Al,Ni}}$ fully relaxed | 246    | 152    | 114    | 218    | 148    | 246    | 61     | 29     | 116    |
| $\Sigma 5(210)^{\text{Al,Ni}}$ interface-constrained | 243    | 146    | 112    | 214    | 152    | 244    | 60     | 25     | 115    |
| Lin. elast. [91] | 278    | 152    | 119    | 246    | 152    | 278    | 127    | 71     | 127    |

The studied $\Sigma 5(210)^{\text{Al,Ni}}$ GB interface states have an orthorhombic symmetry and comparison of sub-figures figure 2a,b based on \emph{ab initio} results obtained for the bulk Ni$_3$Al with those obtained for the $\Sigma 5(210)^{\text{Al,Ni}}$ GB states (figure 2c-f) clearly shows how very different the elasticity of GB states is compared with the bulk (see the impact of other grain boundaries and twins on the Young’s modulus reported in Ref. [92]). The stiffest directions with the Young’s modulus of about 250 GPa are within the same crystallographic plane as the GB interface while the softest directions with the Young’s modulus lower than 90 GPa are inclined to the GB interface plane. When checking the computed elastic constants listed in table 1, it is important to note that the obtained shear elastic constants $C_{44}$ and $C_{55}$ of interface states associated with the $\Sigma 5(210)$ GBs are considerably lower than those in the bulk. In particular, the elastic constant $C_{55}$ is nearly three times lower (29 and 25 GPa) when compared with the bulk value (76 GPa in the same coordination system). To assess these changes and their effect on the mechanical stability, we apply Born and Huang’s stability criteria [80] that connect the mechanical stability with the positiveness of leading principal minors of the matrix of elastic constants. As the diagonal elements $C_{44}$, $C_{55}$ and $C_{66}$ must be positive, the drop predicted for $C_{55}$ clearly identifies the weakest link. Methodologically, it is also important to note that the two different simulation approaches, i.e. full relaxation and the restricted relaxation when the GB interface dimensions in the GB plane are kept equal to the bulk values (as a model for the constraining impact of the underlying grain interior), gave us very similar results (compare the sub-figures 2c,e and 2d,f) as well as the actual values of the elastic constants in table 1.

Our \emph{ab initio} study is devoted to tensorial properties of interface GB states, i.e. to material formed by only a few atomic layers of atoms close to a particular extended defect. In order to study them, the size of the supercells is carefully chosen to contain only a minimum amount of the bulk material (the grain interior; more details may be found in Ref. [63]). Complementarily, we also address another limiting case when we have such a high amount of bulk grain material that the impact of the interface states related to grain boundaries becomes negligible. To do so we employ a linear-elasticity approach derived for coherent multilayers (so-called superlattices) by Grimsditch and Nizzoli [91]. This method processes as the input the tensor of elastic constants for bulk Ni$_3$Al (see the values in table 1) that is rotated [93] by two different angles so as to mimic the rotations of the two interfacing grains which form the studied $\Sigma 5(210)$ GB. The elastic constants obtained in this way essentially correspond to a coherent two-phase multilayer system (stacked along the $z$-axis in our coordinate system). The resulting elastic constants are listed in table 1 and visualized in figure 3 in the form of a directional dependence of the Young’s modulus. We can conclude that the pronounced softening of the Young’s modulus under 100 GPa, which we discussed above in case of the GB states, is not present.
Figure 3. Schematics of the application of the linear elasticity theory by Grimsditch and Nizzoli [91] illustrated by the directional dependencies of the Young modulus (in GPa) of both grains (the directional dependences are rotated in the same way as are rotated the two grains forming the grain boundary) and the combined grain boundary Σ5(210) state (the GBs interface is the x-y plane).

As we have now the complete elastic tensor of Σ5(210)\textsuperscript{Al,Ni} GB state (both fully relaxed and interface-constrained for comparison) we can use the Debye model [94] to access the impact of different elasticities of GB states on some of high-temperature thermodynamic properties of the studied states. In particular, we employ approximative Slater’s approach [82] which was successfully used, e.g., in the case of Ti-Ta alloys as reported in the recently published paper by Chakraborty et al. [95]. In this modeling scheme the Debye temperature Θ\textsubscript{D} is estimated using the following equation:

\[
\Theta_D = \frac{k_B}{\hbar} \left( \frac{6 \pi^2 V^{1/2}}{n} \right)^{1/3} f(\nu) \sqrt{\frac{B_S}{M}},
\]

which is valid for an isotropic solid and, therefore, we will below used integral homogenized elastic characteristics corresponding to a polycrystalline aggregate (which are isotropic). The function \( f(\nu) \) is defined as

\[
f(\nu) = \left\{ 3 \left[ 2 \left( \frac{1 + \nu}{3 - 2\nu} \right)^{3/2} + \left( \frac{1 + \nu}{3 - \nu} \right)^{3/2} \right]^{-1} \right\}^{1/3}
\]
where $\hbar$ is the reduced Planck constant, $k_B$ is the Boltzmann constant, $V$ is molecular volume and mass per formula unit and $M$ is a logarithmically-averaged molecular mass per formula unit containing $n$ atoms. The function $f(\nu)$ depends on the value of the homogenized Poisson’s ratio. The adiabatic bulk modulus $B_S$ we approximate here by the homogenized value of the static bulk modulus $B(V) = V(d^2E(V)/dV^2)$ (as the measure of triaxial compressibility).

Both integral elastic characteristics, the homogenized bulk modulus $B$ and the Poisson ratio, are determined for each set of elastic constants (for the bulk Ni$_3$Al and both fully relaxed and interface-constrained Σ5(210)$^{\text{Al,Ni}}$ GB states, see table 1) by the self-consistent $T$-matrix solution for the effective medium. The $T$-matrix approach is based on the multiple scattering theory and was originally applied to determine elastic properties of single-phase polycrystals with cubic symmetry by Zeller and Dederichs [96]. This concept was generalized by Middya and Basu [97] to the case of single-phase crystals of non-cubic symmetry and further extended by Middya et al. [98] to multi-phase composites. The method is implemented in the SC-EMA [99-101]. The resulting values of the integral (polycrystalline) isotropic Young’s modulus $Y$, bulk modulus $B$ and the Poisson’s ratio as well as the volume $V/V_{\text{bulk}}$ (relative to the bulk) are summarized in table 2.

As the next step, according to the approximative Lindemann’s relation there is a linear connection between the value of the Debye temperature and the melting temperature (see, e.g., Ref. [102]) and we suppose a linear coefficient of this relation to be constant for all studied states. Analyzing equation (1) we can see that in case of the bulk Ni$_3$Al and the prediction of interface states by the linear-elasticity method (a limit of infinitely big grains) the Debye temperature (and thanks to the linear relations also the melting temperature) is predicted to be nearly identical because their molar masses and volumes are identical and their Poisson’s ratios are nearly the same (the differences being caused mostly by numerical rounding errors).

The situation is very different in the case of both quantum-mechanically studied Σ5(210)$^{\text{Al,Ni}}$ GB states. Their molar mass is identical too (the computational supercells are stoichiometric containing an integer number of Ni$_3$Al formula units) but they exhibit very significant changes in the Poisson number $\nu$ and the bulk modulus $B$ (to a lesser extent also those of the volume) which determine the values of the Debye temperature and, subsequently, the melting temperature. The numerical analysis of equation (1) then results in a drastic reduction of the melting temperature to 80.7 % in case of fully-relaxed Σ5(210)$^{\text{Al,Ni}}$ GB state and 78.7 % in case of the interface-constrained one.

**Table 2.** The calculated integral (polycrystalline) isotropic Young’s modulus $Y$ (in GPa), bulk modulus $B$ (in GPa) and the Poisson’s ratio as well as the volume $V/V_{\text{bulk}}$ (relative to the bulk) based on the parameters obtained for (i) the Ni$_3$Al bulk, (ii) Ni$_3$Al Σ5(210)$^{\text{Al,Ni}}$ GBs states (see figure 1a) both fully relaxed and interface-constrained, and (iii) a coherent stack of infinitely big grain assessed by the linear-elasticity approach from Ref. [91].

| Ni$_3$Al states: | $Y$ (in GPa) | $B$ (in GPa) | $\nu$  | $V/V_{\text{bulk}}$ |
|------------------|--------------|--------------|--------|---------------------|
| bulk             | 223          | 183          | 0.2966 | 1.0000              |
| Σ5(210)$^{\text{Al,Ni}}$ fully relaxed | 147          | 172          | 0.3569 | 1.0111              |
| Σ5(210)$^{\text{Al,Ni}}$ interface-constrained | 141          | 169          | 0.3608 | 1.0128              |
| Lin. elast. [91] | 220          | 183          | 0.2996 | 1.0000              |
The above estimated reductions of the melting temperature seem to be too large but it is worth reminding that the studied $\Sigma 5(210)^{\text{Al,Ni}}$ GB state (as computed by the supercell in figure 1a) would model ultra-fined grains with the size of about 1 nm. For these grain sizes, and in the case of nano-particle systems in general, it is known that the melting temperature may be significantly reduced (see, e.g., Ref. [103]). Further, the predicted drop of the melting temperature as a function of the particles size is especially steep for nano-particles smaller than about 10 nm (see the reported reduction to 88% of the melting temperature in case of 5 nm nano-particles in Ref. [104]). Therefore, our predictions have the correct order of magnitude.

4. Conclusions

We have applied quantum-mechanical calculations to estimate high-temperature thermodynamic properties (changes in the melting temperature) of the interface states in Ni$_3$Al associated with the $\Sigma 5(210)$ grain boundary and to determine their tensorial elastic properties. We find the elastic constants of GB states to be very different from those of the bulk Ni$_3$Al and nearly three-fold reduction of the elastic constant $C_{55}$ is identified as the crucial weakest link for the mechanical stability of the studied GB states. Having the complete elastic tensor of $\Sigma 5(210)$ GB states we combine a Green’s-function-based homogenization technique and Slater’s approximative approach to the Debye model to compare thermodynamic properties of a perfect Ni$_3$Al bulk and the $\Sigma 5(210)$ GB states. As a result, significant reduction of the melting temperature (80.7 % and 78.7 % compared with the bulk value) is predicted. Our study thus clearly shows the importance of elastic-constant analysis for, studies of interface states close to GBs when determining their mechanical (in-)stability as well as thermodynamic properties based on ab initio calculations (see, e.g., Refs. [105, 106]). These studies should be ideally extended by phonon spectrum calculations, in-plane translation analysis (see, e.g., Ref. [107]) and simulations of larger deformations (see, e.g., Refs. [108-117]) in the future.

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