**Ab Initio** Study of the Influence of Alloying Elements on Stability and Mechanical Properties of Selected Ti$_x$Al$_y$ Intermetallic Compounds and Their Ti$_x$Al$_y$/Al, Ti$_x$Al$_y$/Ti Interfaces in Explosively Welded Metal–Metal Composites

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The overall performance of joints fabricated using the explosive welding method depends directly on the brittleness of created intermetallic phases and their cohesion with metallic substrates. In this article, we used first principles calculations to show that Sn, V, Cu, and Mg alloying elements present in Ti- and Al-based alloys have a significant influence on the elastic properties and plastic deformation ability of γ-TiAl and Ti$_3$Al. Selected solutes exhibit diversified preferential site occupancy in bulk phases and ordered phase/metallic substrate interface regions. The largest positive effect on ductility and cleavage energy was found for Cu addition (25 pct increase in the B/G ratio), while Sn largely deteriorates cleavage resistance (up to 8 pct). The presented results reveal that further development in the explosive welding field can be reached through the design/application of new alloys composed of elements that improve the properties of the ordered phases present in the joints.

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I. INTRODUCTION

Metal–Metal laminate composites enable the attractive functional properties and high strength of two different materials to be combined. Such complex solutions offer unique properties that are often unachievable in single metals. [1] The most widely used industrial method of production of layered metal composites is explosive welding, where the single-step process forms bimetallic joints. [2,3] However, the typical conditions of the method, i.e., extremely high strain rates (collision point velocity up to 4500 m/s [4]) and local heating (in the range of 2500 K [5]) promote a sophisticated structure of the welded zone with an extensively deformed region and brittle phases. [3] This type of interface microstructure was observed in numerous laminates composed of pure Ti and Al [6–10] as well as those formed from Ti, Al, Fe, and Ni alloys. [11–13] According to available reports, the crucial structural aspect of interface strength is related to the type and number of ordered phases acting as the crack nucleation and propagation region. Moreover, recent studies of Ti–Al and Ti–Fe explosive joints indicate that intermetallic inclusions form a thin, continuous layer at the interface with a non-homogeneous shape and chemical stoichiometry. [7,13] To date, considerable effort has been made to minimize the negative effect (brittleness) of these intermetallic systems, through annealing or hot rolling. [7,14–16]

Another way to improve the properties of joints is to alloy the existing intermetallic phases to enhance their ductility and the cohesion of their phase boundaries. Improving the room temperature ductility of the ordered structures through alloying has been extensively explored over recent decades, leading to marked achievements arising from three separate mechanisms [17,18]: (i) the activation of new, or the facilitation of, the original dislocation slip modes; (ii) the segregation of solutes at grain boundaries, increasing their cohesion and limiting intergranular fracture; and (iii) the reconfiguration of the base, brittle crystal lattice to achieve higher symmetry and more ductile structures. These strategies were adopted for various intermetallic systems, e.g., NiAl alloyed with Fe or Mn exhibits large ductility improvement caused by lattice expansion induced by the magnetic coupling between solute and host atoms reducing the shear modulus and generalized stacking fault energy of $\{11\{110\}$ slip mode. [19–21] Nb
addition to Ti₃Al phase activates 1120(0001) basal slip, which is absent in unalloyed material,\cite{22} segregation of interstitial boron in Ni₅Al grain boundaries increase their cohesion and minimize intergranular cleavage;\cite{17,23,24} although, alloying with some substitutional elements (Zr, Hf, V, Nb, Mo, W, Co, Pd, Cu, Cr, Mn, and Fe) increases overall ductility of this phase as well;\cite{24}

As can be seen from the reviewed literature, the addition of the ternary element to the binary intermetallic phase can significantly improve its deformation ability. This behavior can be potentially utilized in the explosive welding method to reduce the detrimental effect of ordered structures formed at the interface area. However, to this end, a careful selection of alloying elements has to be made. As explosive welding is already a commercial technology, it is worth first investigating the effect of solutes present in commercial alloys. Such an approach is highly desirable from an industrial point of view, in order to identify materials whose joints may be less brittle. In this article, we follow the above idea and adopt \textit{ab initio} modeling to explore the influence of solutes present in Ti and Al alloys on the mechanical properties (elastic constants, $B/G$ Pugh plasticity criterion)\cite{23} of Ti₃Al and $\gamma$-TiAl, as well as the cleavage energy of selected interfaces between these phases and both metallic substrates at 0 K temperature.

We consider four substitutional solutes, i.e., Sn, V, Cu, and Mg, prevalent in a number of Ti (Ti-6Al-4V, Ti-3Al-2.5V, Ti-10V-2Fe-3Al, Ti-15V-3Cr-3Sn-3Al, Ti-11Sn-5Zr-2.25Al-1Mo-0.2Si, Ti-6Al-2Sn-4Zr-2Mo-0.08Si\cite{26}) or Al (Aluminum series 2XXX and 5XXX\cite{27}) commercial alloys.

II. METHODOLOGY

The \textit{ab initio} calculations were performed with a Vienna \textit{ab initio} Simulation Package (VASP) code,\cite{28,29} using the projector augmented wave (PAW) technique\cite{30} and a Perdew–Burke–Ernzerhof generalized gradient functional.\cite{31} The 0.2 eV smearing of electronic occupancy was approximated with a Methfessel–Paxton electronic wave function close to the energy minimum. The simulation boxes utilized for elastic constants calculations were created using the supercell approach,\cite{32,33} with Reuss–Hill approximation\cite{41–43}: the elastic constants

$$E(V, \varepsilon) = E_0 + V_0 \sum_{i=1}^{6} \sigma_i e_i + \frac{1}{2} \sum_{i,j=1}^{6} C_{ij} e_i e_j,$$  

where $E$ is the total energy (including all electrostatic interactions, exchange correlation and kinetic energy of the electrons, as well as energy of the ions in the PAW approach) of the elastically distorted crystal, $E_0$ and $V_0$ are the total energy and volume of the system in its ground state, and $\sigma_i$, $e_i$ are the stress and strain tensors, respectively, written in Voigt notation. In the approach above, the elastic constants are extracted by fitting the total energies derived under different strains to quadratic function close to the energy minimum. The six and five independent elastic constants of tetragonal $\gamma$-TiAl and hexagonal Ti₃Al, respectively, were determined with the distortions $D_i$ given in Table I ($C_{66} = (C_{11} - C_{12})/2$ for Ti₃Al).\cite{35,40} Having $C_{ij}$ it is possible to calculate the polycrystalline shear $G$, bulk $B$, and Young $E$ moduli of the studied phases with Reuss–Hill approximation\cite{41–43}:

$$B = \frac{B_V + B_R}{2},$$

$$G = \frac{G_V + G_R}{2},$$

$$E = \frac{9BG}{3B + G},$$

where $B_V$, $G_V$, $B_R$, and $G_R$ are Voigt and Reuss bulk and shear moduli obtained by
The final evaluation of the brittle/ductile nature of investigated phases is quantified based on the $B/G$ Pugh plasticity criterion, originally proposed for pure metals\(^\text{[25]}\) and later used for a wide group of compounds with complex structures and diversified stoichiometry.\(^\text{[44]}\) The considered intermetallic phases exhibit a metallic nature (no band gap,\(^\text{[45]}\) good electrical conductivity\(^\text{[46,47]}\)). As the constituent elements are simple (Al) and transition (Ti) metals, the bond character is mixed, metallic (s and p-type electrons), and covalent (d-type electrons). For such systems, the transition from brittle cleavage to ductile failure of the material occurs at $B/G = 1.75$. This critical value should not be viewed as a definitive transition point, as the criterion fails to capture the entire complexity of such a transition. Nevertheless, the higher the $B/G$ the larger the expected ability of the material to undergo plastic deformation.

III. RESULTS AND DISCUSSION

A. Solute Site Occupancy and Mechanical Properties

To determine the preferential site of solutes (Ti- or Al-sublattice) in $\gamma$-TiAl and Ti$_3$Al phases, the average formation energy $E_f$ has been calculated according to

$$E_f = \frac{E_{\text{tot}} - n_{\text{Ti}}E_{\text{Ti solid}} - n_{\text{Al}}E_{\text{Al solid}} - E_X}{N},$$

where $E_{\text{tot}}$ is the total energy of alloyed $\gamma$-TiAl or Ti$_3$Al structures composed of $n_{\text{Ti}}$ and $n_{\text{Al}}$ numbers of Ti and Al atoms; $E_{\text{Ti solid}}$, $E_{\text{Al solid}}$, and $E_X$ are energy per atom of Ti, Al, and solute element in their reference, stable states, respectively. The total number of atoms in the simulation box is denoted as $N$ (in this study, $N = 16$). Negative formation energy indicates that the solute prefers to dissolve in the intermetallic phase rather than forming separate pure structures. The lower the $E_f$ the larger the structural stability of the given configuration at 0 K. The calculated $E_f$ are presented in Table II, which shows that Cu and Sn occupy the Al site in $\gamma$-TiAl, while Mg and V are located at the Ti sublattice. On the other hand, in the case of Ti$_3$Al for all of the investigated solutes except Sn, the Ti site is the lower energy one. The preferential occupancy of the Al site by Sn in Ti$_3$Al can be clarified by the presence of Ti$_3$Sn compound with an analogous configuration to Ti$_3$Al.\(^\text{[50]}\) The available experiments confirm the determined site occupancies for V and Sn in $\gamma$-TiAl and Ti$_3$Al also at room temperature,\(^\text{[51]}\) and indicate good solubility of transition and simple metals in these structures, at least up to 5 at. pct.\(^\text{[52]}\)

Knowing the preferential site occupancy of substitutional solutions, the elastic constants of both pure and alloyed $\gamma$-TiAl and Ti$_3$Al were calculated and are listed in Table III. It can be found that $B$ and $G$ values...
determined in this work predict the properties of materials at 0 K temperature. The highest error relative to low temperature experiments reaches 4 and 8 GPa for B and G, respectively. It is worth noting that, according to experimental data, these moduli are relatively constant between 0 K and 298 K, with the largest change equal to 5.1 pct \((G \text{ of Ti}_3\text{Al})\). The \(B/G\) plasticity criterion agrees reasonably well with the available experiments and other theoretical data. Some discrepancy between calculated elastic constants results from different pseudopotential approaches and computational parameters used by different authors. Considering the alloyed systems, it can be found that elements of the \(C_{ij}\) matrix change significantly for both phases, leading to noticeable variations of \(B/G\). The addition of Mg or Sn enhances the brittleness, while V merely affects the Pugh plasticity criterion.\[^7\] Investigated \(E_i\) has a similar physical meaning to \(E_i\) from Eq. \([10]\), i.e., \(E_i\) describes the formation energies of solutes located close to the interface at 0 K, thus, negative \(E_i\) indicates the (meta-)stable position of a given element. Lattice vibrations existing at finite temperatures may also influence the most favorable location of particular alloying elements, when \(E_i\) is similar for different configurations. In this study, we selected seven interfaces, Ti3Al (0001) || Al (111), Ti3Al (0001) || Ti (0001), Ti3Al (1010) || Ti (1010), \(\gamma\)-TiAl (001) || Al (001), \(\gamma\)-TiAl (100) || Al (100), \(\gamma\)-TiAl (111) || Al (111), \(\gamma\)-TiAl (111) || Ti (0001), which include different types of crystallographic planes between Ti–Al compounds and Ti- or Al-substrates, and various distributions of constituent elements. The selected interfaces are coherent with the maximum misfit strains up to 4 pct, as listed in Table IV. According to recent reports, the interaction of alloying elements with 2D defects depends non-linearly on their relative distance.\[^61\] This effect arises from the local relaxation of atomic positions, lattice misfit strains, and 3D perturbation of electronic structure present in the thin region above and below the planar imperfections of the crystal structure. In view of the above phenomenon, the \(E_i\) was calculated for six positions of solutes, i.e., the three closest to the interface atomic planes from both intermetallic and substrate sites, as shown in Figure 2. Furthermore, depending on the interface type, alloying elements can also occupy Ti or Al position in the same atomic plane. The determined \(E_i\) reveals that Mg is the only insoluble element in the investigated interfaces, while Sn and V can occupy numerous metastable (with negative but not the lowest segregation energy) positions on both the intermetallic and metallic parts of the crystals. Cu displays moderate \(E_i\) values, exhibiting a relatively low structural stability in most cases. Another important result is related to the preferential Ti or Al site of solutes in ordered phases. According to Table II, V occupies the position of Ti atoms in both bulk \(\gamma\)-TiAl and Ti3Al structures, while closer to the interfaces, a more stable configuration can be changed to an Al sublattice, as in \(\gamma\)-TiAl (100) || Al (100), \(\gamma\)-TiAl (111) || Al (111) systems (Figure 3).

To reveal the effect of solute atoms on the strength of \(\gamma\)-TiAl(Ti3Al)/Ti(Al) interfaces, the \(\gamma\)-c cleavage energy of

\[
E_{\text{TiAl}} = u_{\text{Ti}} + u_{\text{Al}} \quad [12]
\]

and

\[
E_{\text{Ti3Al}} = 3u_{\text{Ti}} + u_{\text{Al}}, \quad [13]
\]

where \(E_{\text{TiAl}}\) and \(E_{\text{Ti3Al}}\) are the total energies of \(\gamma\)-TiAl and Ti3Al unit cells. Such obtained chemical potentials \((u_{\text{Ti}} = -8.05 \text{ eV and } u_{\text{Al}} = -4.40 \text{ eV agree well with the available theoretical data: } u_{\text{Ti}} = -7.89 \text{ eV and } u_{\text{Al}} = -4.46 \text{ eV calculated at 0 K temperature in Reference 60})\) correspond to the two-phase field of Ti and Al phase diagram, which is typically obtained in the welded Ti/Al joints, i.e., \(\gamma\)-TiAl, Ti3Al as well as non-stoichiometric compositions of intermetallic phases occur in the direct mutual vicinity.\[^7\] Investigated \(E_i\) has a similar physical meaning to \(E_i\) from Eq. \([10]\), i.e., \(E_i\) describes the formation energies of solutes located close to the interface at 0 K, thus, negative \(E_i\) indicates the (meta-)stable position of a given element. Lattice vibrations existing at finite temperatures may also influence the most favorable location of particular alloying elements, when \(E_i\) is similar for different configurations. In this study, we selected seven interfaces, Ti3Al (0001) || Al (111), Ti3Al (0001) || Ti (0001), Ti3Al (1010) || Ti (1010), \(\gamma\)-TiAl (001) || Al (001), \(\gamma\)-TiAl (100) || Al (100), \(\gamma\)-TiAl (111) || Al (111), \(\gamma\)-TiAl (111) || Ti (0001), which include different types of crystallographic planes between Ti–Al compounds and Ti- or Al-substrates, and various distributions of constituent elements. The selected interfaces are coherent with the maximum misfit strains up to 4 pct, as listed in Table IV. According to recent reports, the interaction of alloying elements with 2D defects depends non-linearly on their relative distance.\[^61\] This effect arises from the local relaxation of atomic positions, lattice misfit strains, and 3D perturbation of electronic structure present in the thin region above and below the planar imperfections of the crystal structure. In view of the above phenomena, the \(E_i\) was calculated for six positions of solutes, i.e., the three closest to the interface atomic planes from both intermetallic and substrate sites, as shown in Figure 2. Furthermore, depending on the interface type, alloying elements can also occupy Ti or Al position in the same atomic plane. The determined \(E_i\) reveals that Mg is the only insoluble element in the investigated interfaces, while Sn and V can occupy numerous metastable (with negative but not the lowest segregation energy) positions on both the intermetallic and metallic parts of the crystals. Cu displays moderate \(E_i\) values, exhibiting a relatively low structural stability in most cases. Another important result is related to the preferential Ti or Al site of solutes in ordered phases. According to Table II, V occupies the position of Ti atoms in both bulk \(\gamma\)-TiAl and Ti3Al structures, while closer to the interfaces, a more stable configuration can be changed to an Al sublattice, as in \(\gamma\)-TiAl (100) || Al (100), \(\gamma\)-TiAl (111) || Al (111) systems (Figure 3).

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\]
Table I. Crystal Distortions $D_x$ Used to Calculate the Elastic Constants and Corresponding Coefficients of the Second Degree Variable of the Parabolic Fit of Energy Variations at the Applied Strain State

| Structure       | Distortion                                                                 | $\frac{1}{V_0} \frac{\partial^2 E(V, \epsilon)}{\partial \epsilon^2} \bigg|_{\epsilon=0}$ |
|-----------------|----------------------------------------------------------------------------|--------------------------------------------------------------------------------|
| $\gamma$-TiAl   | $D_1 = \begin{pmatrix} 1 + \epsilon & 0 & 0 \\ 0 & 1 + \epsilon & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $C_{11} + C_{12}$                                                                  |
| ($L1_0$)        | $D_2 = \begin{pmatrix} 1 + \epsilon & 0 & 0 \\ 0 & 1 + \epsilon & 0 \\ 0 & 0 & 1 + \epsilon \end{pmatrix}$ | $C_{11} + C_{12} + 2C_{33} - 4C_{13}$                                              |
| $\gamma$-TiAl   | $D_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 + \epsilon \end{pmatrix}$ | $4C_{44}$                                                                        |
| ($L1_0$)        | $D_4 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 + \epsilon & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $2C_{66}$                                                                        |
| $\gamma$-TiAl   | $D_5 = \begin{pmatrix} 1 & 0 & \epsilon \\ \epsilon & 1 + \epsilon & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $\frac{1}{2}(2C_{11} + 2C_{12} + 4C_{13} + C_{33})$ |
| ($L1_0$)        | $D_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 + \epsilon & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $C_{11} + C_{12}$                                                                  |

Table II. The Formation Energies (Eq. [10]) Calculated for Pure and Alloyed $\gamma$-TiAl and Ti$_3$Al (Solute Concentration 6.25 At. Pct)

| Structure       | $E_f$—Ti Site | $E_f$—Al Site | Solute Preferred Site |
|-----------------|---------------|---------------|-----------------------|
| $\gamma$-TiAl + Cu | -0.361        | -0.367        | Al                    |
| $\gamma$-TiAl + Mg | -0.353        | -0.326        | Ti                    |
| $\gamma$-TiAl + Sn | -0.341        | -0.393        | Al                    |
| $\gamma$-TiAl + V  | -0.382        | -0.368        | Ti                    |
| $\gamma$-TiAl     | -0.408, $0.416^{[48]}$, $0.449^{[33]}$, -        | -                      | —                     |
|                  | 0.401$^T$[49] | -                      | —                     |
| Ti$_3$Al + Cu     | -0.248        | -0.198        | Ti                    |
| Ti$_3$Al + Mg     | -0.227        | -0.173        | Ti                    |
| Ti$_3$Al + Sn     | -0.279        | -0.284        | Al                    |
| Ti$_3$Al + V      | -0.261        | -0.178        | Ti                    |
| Ti$_3$Al          | -0.282, $0.256^{[48]}$, $0.279^T$[49] | -                      | —                     |

The “E” and “T” superscript symbols indicate the reference experimental and theoretical data, respectively. $E_f$ given eV/atom.
pure and most stable alloyed systems (configurations with the lowest $E_s$ from Figure 2) was calculated using the following equation:

$$\gamma_c = \frac{E_{\text{lab}}^{\text{TiAl}}}{}$$

and

Table III. The Single Crystal and Polycrystalline Elastic Constants of Pure and Alloyed $\gamma$-TiAl and Ti$_3$Al (Solute Concentration 6.25 At. Pct)

| Structure          | $C_{11}$ | $C_{12}$ | $C_{13}$ | $C_{33}$ | $C_{44}$ | $C_{66}$ | $B$   | $G$  | $E$  | $B/G$ |
|--------------------|----------|----------|----------|----------|----------|----------|-------|------|------|-------|
| $\gamma$-TiAl      | 202.9    | 58.3     | 87.7     | 174.4    | 112.7    | 43.2     | 116.4 | 70.5 | 176.0 | 1.65  |
| $\gamma$-TiAl      | 110$^{[53]}$ | 74$^{[53]}$ | 181.5$^{[53]}$ | 1.49$^{[53]}$ |
| Ti$_3$Al           | 79.7     | 78.3$^{[54]}$ | 185$^{[54]}$ | 1.45$^{[54]}$ |
| (0 K)              | 110$^{[54]}$ | 78.3$^{[54]}$ | 176$^{[54]}$ | 1.45$^{[54]}$ |
| 112$^{[54]}$       | 78.3$^{[54]}$ | 176$^{[54]}$ | 1.45$^{[54]}$ |
| $\gamma$-TiAl + Cu | 178.6    | 75.1     | 102.9    | 157.3    | 108.8    | 37.6     | 119.6 | 56.7 | 149.0 | 2.07  |
| $\gamma$-TiAl + Mg | 194.9    | 42.9     | 78.6     | 158.3    | 101.8    | 44.0     | 105.4 | 67.4 | 166.7 | 1.56  |
| $\gamma$-TiAl + Sn | 212.8    | 59.1     | 75.8     | 192.4    | 104.7    | 43.7     | 115.5 | 73.7 | 182.2 | 1.57  |
| $\gamma$-TiAl + V  | 216.2    | 52.9     | 88.9     | 182.2    | 115.3    | 36.8     | 119.5 | 71.4 | 178.7 | 1.67  |
| Ti$_3$Al           | 199.7    | 89.3     | 61.1     | 231.9    | 64.6     | 55.2     | 117.1 | 64.0 | 162.4 | 1.83  |
| $\gamma$-TiAl      | 199.7    | 89.3     | 61.1     | 231.9    | 64.6     | 55.2     | 117.1 | 64.0 | 162.4 | 1.83  |
| $\gamma$-TiAl + Cu | 177.0    | 94.0     | 70.8     | 210.1    | 45.8     | 41.5     | 116.1 | 55.8 | 144.4 | 2.08  |
| $\gamma$-TiAl + Mg | 177.5    | 84.0     | 66.0     | 206.7    | 64.2     | 46.7     | 113.8 | 60.6 | 154.8 | 1.88  |
| $\gamma$-TiAl + Sn | 189.4    | 92.2     | 67.0     | 223.3    | 57.5     | 48.6     | 117.1 | 60.5 | 154.8 | 1.94  |
| $\gamma$-TiAl + V  | 198.1    | 93.4     | 65.5     | 239.5    | 58.9     | 52.4     | 118.8 | 62.3 | 159.1 | 1.91  |

The “E” and “T” superscript symbols indicate the reference experimental and theoretical data, respectively. Please note that $C_{ij}$ elements are determined for BCT representation of $\gamma$-TiAl.$^{[32,33]}$ The theoretical data correspond to 0 K and all the results given in GPa.

Table IV. Misfit Strains Measured for the Directions Parallel to the Subsequent Interfaces

| Interface          | Phase and Direction | Dimension (Å) | Misfit Strain (pct) |
|--------------------|---------------------|---------------|---------------------|
| $\gamma$-TiAl(001) || Al(001)           | $\gamma$-TiAl [010] | 3.995             | 1.7                |
|                    |                     | Al [010]      | 4.061              | 1.6                |
| $\gamma$-TiAl(100) || Al(100)           | $\gamma$-TiAl [010] | 3.995             | 1.7                |
|                    |                     | Al [010]      | 4.061              | 1.6                |
| $\gamma$-TiAl(111) || Al(111)           | $\gamma$-TiAl [011] | 4.535             | 0.2                |
|                    |                     | Al [011]      | 5.703              | 0.1                |
| $\gamma$-TiAl(111) || Ti(0001)          | $\gamma$-TiAl 1/2[011] | 2.852             | 2.9                |
|                    |                     | Ti [1120]     | 2.936              | 2.9                |
| Ti$_3$Al(0001)    || Al(111)           | Ti$_3$Al [1120] | 2.824             | 0.9                |
|                    |                     | Al 1/2 [011]  | 2.849              | 0.9                |
| Ti$_3$Al(0001)    || Ti(0001)          | Ti$_3$Al [1120] | 2.824             | 0.9                |
|                    |                     | Ti [1120]     | 2.936              | 3.8                |
| Ti$_3$Al(1010) || Ti(1010)          | Ti$_3$Al [1120] | 2.824             | 0.9                |
|                    |                     | Ti [1120]     | 2.936              | 3.8                |
|                    |                     | Ti$_3$Al [0001] | 4.655             | -0.02              |
|                    |                     | Ti [0001]     | 4.648              | 0.02               |

Depending on the lattice symmetry, particular systems exhibit two independent misfit strains along two perpendicular crystallographic directions. The listed dimensions were calculated for defect-free structures.
\[
\gamma_{TiAl}(001) \parallel Al(001) \quad \gamma_{TiAl}(100) \parallel Al(100) \quad \gamma_{TiAl}(111) \parallel Al(001) \quad Ti_{3}Al(1010) \parallel Ti(1010)
\]

Fig. 2—Examples of the investigated \(\gamma\)-TiAl(\(Ti_{3}Al\))/Ti(Al) interfaces. The analyzed positions of solutes lying on six (\(\ldots 3, 2, \ldots, 3\)) closest to the interface atomic planes are marked by black squares. The Ti and Al atoms are denoted by blue and gray, respectively (Color figure online).

\[
\gamma_{c} = E_{slab}^{Ti(Al)} + E_{slab}^{Ti(Al)\ldots Ti(Al)\ldots Ti(Al)\ldots Ti(Al)} - E_{slab}^{Ti_{3}Al(0001)\parallel Ti(0001)}
\]

where \(E_{slab}^{Ti(Al)}\) and \(E_{slab}^{Ti(Al)\ldots Ti(Al)\ldots Ti(Al)\ldots Ti(Al)}\) are the total energies of the 6-layer, pure Ti (or Al) and TiAl (or \(Ti_{3}Al\)) crystals, \(E_{slab}^{Ti(Al)/Ti(Al)}\) is the total energy of the 12-layer, interface-involved structures composed of the same Ti (or Al) and TiAl (or \(Ti_{3}Al\)) systems and \(A\) is the interface area. For alloyed configurations, \(E_{slab}^{Ti(Al)/Ti(Al)/Ti_{3}Al\ldots X}\) and \(E_{slab}^{Ti(Al)/Ti(Al)/Ti_{3}Al\ldots X}\) denote the total energies of the 6-layer Ti, Al, TiAl, or \(Ti_{3}Al\) enriched by one solute element and pure crystals, respectively. The final \(E_{slab}^{Ti(Al)/Ti(Al)/Ti(Al)/X}\) term is the total energy of the alloyed, 12-layer \(\gamma_{TiAl}(Ti_{3}Al)/Ti(Al)\) structure. It should be noted that, due to periodic boundary conditions, the original interface-involved models (Figure 1) were transformed to slab structures by adding an 8 Å vacuum region in each case (the size of the 6- and corresponding 12-layer simulation boxes was always equal, to ensure the same density of k-points). According to Eqs. [14] and [15], \(\gamma_{c}\) is the energy per unit area required to separate the solid into two semi-infinite blocks, creating two free surfaces. \(^{60,62}\) The calculated \(\gamma_{c}\) of pure and alloyed \(\gamma_{TiAl}(Ti_{3}Al)/Ti(Al)\) interfaces are presented in Table V, and the investigated systems are listed in terms of increasing cleavage energy: \(\gamma_{TiAl}(111)\parallel Al(111) < \gamma_{TiAl}(100)\parallel Al(100) < \gamma_{TiAl}(0001)\parallel Al(0001) < \gamma_{TiAl}(111)\parallel Al(111) < \gamma_{TiAl}(0001)\parallel Al(0001) < \gamma_{TiAl}(0001)\parallel Ti(0001) < \gamma_{TiAl}(0001)\parallel Ti(0100) < \gamma_{TiAl}(0100)\parallel Ti(1010).\)

The gathered data illustrate a pronounced difference in the strength of interfaces formed between the analyzed phases. The strongest (the highest \(\gamma_{c}\)) systems are those containing the largest fraction of Ti atoms, which, thanks to d-type electrons, form more directional, covalent bonds. \(^{38,63}\) The addition of solute atoms, overall, leads to relatively small changes of
cleavage energy. However, the absolute values of $\gamma_c$ variations are comparable to the influence of alloying elements on the energy of other types of 2D defects, the stacking faults.\[61,64\]

To gain a better understanding of the influence of solute atoms on cleavage energy, the electronic structure of two alloyed interfaces with the largest variations of $\gamma_c$, i.e., $\gamma$-TiAl (100) || Al (100) + V, Sn and Ti$_3$Al (0001) || Ti (0001) + Sn, Cu is investigated using the electron localization function (ELF) describing the probability of finding two electrons with the same spin in space.\[65–68\] ELF is normalized to the range of 0 to 1, where 0.5 indicates a homogeneous electron gas, whereas values close to 1 represent a highly localized covalent or ionic interactions. As shown in Figures 4(a) and (c), the vanadium atom located close to the $\gamma$-TiAl (100) || Al (100) interface significantly increases the ELF, forming a strong covalent bond with the neighboring Al atoms and increasing $\gamma_c$. On the other hand, the preferential position of Sn is more distant from this planar defect (Figures 4(b) and (d)) and its impact on $\gamma_c$ is low. It should also be noted that the bonds formed by Sn exhibit a different character. Although the localization of electrons around Sn is pronounced, covalent bonds characterized by a local and directional increase in ELF surrounded by ELF depletion\[63,69\] are not formed. Such a topology of ELF function (a closed shell around an ion) corresponds to electrostatic, ionic-like interactions with adjacent atoms. In the case of Ti$_3$Al (0001) || Ti (0001), the addition of Cu (Figures 4(e) and (g)) results in considerable, mixed metallic-covalent bonding visible as an extended, partially directional ELF distribution with moderate value.

For this composition, the $\gamma_c$ is lower than in an unalloyed system, as the amount of original covalent bonds is reduced. The Sn forms again, mainly with electrostatic interaction (Figures 4(f) and (h)) leading to the lowest $\gamma_c$.

IV. CONCLUSIONS

In this article, systematic, first principles calculations were performed to investigate the effect of Sn, V, Cu, and Mg alloying elements on the mechanical properties and structural stability of $\gamma$-TiAl and Ti$_3$Al intermetallic phases present in Ti/Al laminates fabricated with the explosive welding method. Apart from the bulk structures, seven ordered phase/metallic substrate interfaces were analyzed in terms of solutes segregation and cleavage resistance. The gathered data include low temperature (0 K) single- and polycrystalline elastic constants, $B/G$ plasticity criterion, as well as the formation and cleavage energies of the studied systems. It was found that the effect of selected alloying elements is pronounced, especially for the elastic moduli and brittle/ductile behavior of $\gamma$-TiAl and Ti$_3$Al. The presented results can be useful for the proper selection of alloys used in explosive welding techniques and in future simulations extended by temperature effects or detailed plasticity analysis, such as dislocation modeling. The main findings of this work are as follows:

1. Sn, V, Cu, and Mg at 6.25 at. pct concentration are able to dissolve in $\gamma$-TiAl and Ti$_3$Al with negative formation energy.

| Interface Type          | Element | Preferential site | Sublattice | Solute position (lattice plane) | $\gamma_c$ [mJ/m$^2$] |
|-------------------------|---------|-------------------|------------|--------------------------------|------------------------|
| $\gamma$-TiAl (001) || Al (001) | Sn | $\gamma$-TiAl | Al | — 2 | 1957 |
|                        | V       | Al                | Al         | 2 | 2006 |
|                        | Cu      | Al                | Al         | 2 | 1945 |
| $\gamma$-TiAl (100) || Al (100) | Sn | $\gamma$-TiAl | Al | — 3 | 1349 |
|                        | V       | Al                | Al         | 3 | 1338 |
|                        | Cu      | $\gamma$-TiAl     | Al         | 1 | 1420 |
| $\gamma$-TiAl (111) || Al (111) | Sn | $\gamma$-TiAl | Al | — 3 | 1317 |
|                        | V       | Al                | Al         | 3 | 1322 |
|                        | Cu      | $\gamma$-TiAl     | Al         | 1 | 1351 |
| $\gamma$-TiAl (111) || Ti (0001) | Sn | Ti | Ti | 2 | 1820 |
| Ti$_3$Al (0001) || Al (111) | Sn | Ti$_3$Al | Al | — 3 | 1553 |
|                        | V       | Al                | Al         | 3 | 1549 |
|                        | Cu      | Al                | Al         | 3 | 1551 |
| Ti$_3$Al (0001) || Ti (0001) | Sn | Ti | Ti | 1 | 3909 |
|                        | Cu      | Ti                | Ti         | 1 | 3587 |
|                        |         |                   |            |    | 3779 |
| Ti$_3$Al (1010) || Ti (1010) | Sn | Ti | Ti | 1 | 3941 |
|                        | Cu      | Ti                | Ti         | 1 | 3653 |
|                        |         |                   |            |    | 3829 |

The particular positions of alloying elements are indicated by preferential sites relative to the interface ($\gamma$-TiAl, Ti$_3$Al or Ti, Al), sublattice occupation, and distance to interface expressed in the next nearest lattice plane.
2. V and Mg always occupy the Ti sublattice, while Sn tends to substitute Al atoms. Cu prefers the Al and Ti position in γ-TiAl and Ti₃Al, respectively.
3. All the analyzed alloying elements increase the ductility of Ti₃Al, while Mg and Sn enhance the brittle nature of γ-TiAl.
4. Cu increases the B/G Pugh ratio of γ-TiAl and Ti₃Al by 25 and 14 pct, respectively. The above changes make this element a potentially universal solute in terms of the ductility improvement of the studied intermetallic compounds.
5. The investigation of seven selected γ-TiAl(Ti₃Al)/Ti(Al) interfaces showed that Mg is always insoluble close to 2D defects and only Sn is energetically stable at all the interfaces.
6. Solute elements have a noticeable effect on the mechanical properties of the intermetallic phases formed in the joints. Accordingly, the overall strength of the welded systems can be improved by careful selection of the composition of the substrate materials.

Fig. 4.—The electron localization function of the selected alloyed interface with the largest cleavage energy variation: γ-TiAl (100) || Al (100) + V on (a) and (c), γ-TiAl (100) || Al (100) + Sn on (b) and (d), Ti₃Al (0001) || Ti (0001) + Cu on (e) and (g), Ti₃Al (0001) || Ti (0001) + Sn on (f) and (h). Cross-section planes are given below each ELF map. Ti, Al, and solute atoms are denoted by blue, gray and red, respectively. The interface plane is denoted by a black dashed line (Color figure online).
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CONFLICT OF INTEREST

On behalf of all authors, the corresponding author states that there is no conflict of interest.

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