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Original article

Effect of Si and Ti_5Si_3 on the adhesion at the α-Al_2O_3/γ-TiAl interface and oxygen diffusion in the alloy

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ABSTRACT The effect of silicon and Ti_5Si_3 films on the adhesion properties of the α-Al_2O_3/γ-TiAl interface and oxygen diffusion in TiAl was studied using the projector augmented-wave method within density functional theory. It was shown that the formation of intermediate silicide layers at the oxide–alloy interface can lead to a significant decrease in the oxygen diffusion coefficient. At the same time, adhesion at the oxide–silicide interface remains high, while for the silicide–alloy interface, the values of $\sim$2.26–2.80 J/m^2 typical for interfaces with metallic and metal-covalent bonds were obtained.

KEYWORDS titanium aluminides, titanium silicide, oxygen diffusion, adhesion, the ab-initio calculations

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1. Introduction

The structural and physicochemical properties of metal–oxide interfaces have been intensively studied for almost three decades due to their practical and fundamental importance, but they remain the focus of both experimental and theoretical studies [1–3]. It is known that the mechanical properties of composite materials depend significantly on the structure and composition of the interfaces. The formation of interfaces with good mechanical properties is due to a strong chemical bond at the interface, and the degree of compatibility of the crystal lattices of the metal and oxide plays an important role. Knowledge of the electronic structure is necessary to understand the mechanisms of chemical bonding at interfaces. One of the key quantities for describing the mechanical properties of interfaces is the ideal adhesion energy or the work of separation (W_{sep}) [4]. It is defined as the energy that needs to separate the interface into two free surfaces. It is believed that this fundamental quantity determines the strength of interfaces.

It is known that during oxidation of the doped γ-TiAl, a complex intermediate structure can form at the internal interface due to segregation of impurities to the interface and formation of their oxides and other compounds [5–7]. During diffusion of nitrogen from the external environment, titanium nitride films forms, which can be an effective barrier to oxygen penetration into the alloy according to experimental and theoretical studies [8, 9]. Recently, the formation of titanium silicide film was also found at the interface with the TiAl doped by silicon [10, 11], the role of which in increasing the corrosion resistance of TiAl based alloys is ambiguous. It is believed that the formation of the titanium silicide films prevents further oxidation of the alloy. However, the role of the intermediate structure of the interfaces from the point of view of changing both the interface strength and the oxygen diffusion coefficient interface has practically not been studied by theoretical methods. Currently, there are only several papers in which the effect of the so-called buffer layers on the chemical bond at the oxide–metal (alloy) interfaces were studied [12] and references therein. In [13, 14], we estimated the adhesion at the TiAl(111)/Al_2O_3(0001) and TiAl(111)/TiO_2(110) interfaces. The highest values of W_{sep} were obtained for TiAl(111)/$Al_2O_3(0001)_O$ contact with an oxygen termination of the oxide surface (9.97–10.43 J/m^2 [13]), whereas the W_{sep} values at the interface with titanium dioxide were significantly lower (1.97–2.44 J/m^2 [14]). In this work, we studied the effect of silicon and titanium silicide film of the composition Ti_5Si_3 on the adhesion at the TiAl(111)/$Al_2O_3(0001)_O$ interface, as well as the diffusion of oxygen into the alloy.

2. Computational details

The electronic structure of ideal TiAl(111)/$Al_2O_3(0001)_O$ interface was calculated using the projector augmented-wave method [15, 16] with a generalized gradient approximation for the exchangecorrelation functional in the form of PBE–GGA [17]. The energy cutoff for the plane-wave basis set was 550 eV. Integration over the Brillouin zone was performed using a 3×3×1 Γ-centered k-point grid. The interface was modeled using the slab approach with a vacuum gap of $\sim$15 Å thickness. The positions of the atoms in the interface layers were relaxed until the forces on the atoms did not exceed 0.01 eV/Å. The following surface cells were used for the interface modeling: Al_2O_3(0001)-(2×2) and TiAl(111)-($\sqrt{3} \times \sqrt{3}$)$R30°$. The difference between the surface parameters of the oxide and alloy (9.616 Å and 9.826 Å) does not exceed $\sim$2.2%. The lattice parameter of the oxide was used in the calculations. Each atomic layer of the alloy has a stoichiometric composition and is formed by six titanium atoms and six aluminum atoms. The computational cell contained 124 atoms. For estimation of W_{sep} a standard equation from [4] was used.

3. Results and discussion

3.1. Effect of Si and Ti_5Si_3 on the interface adhesion

The interface atoms of aluminum in the γ-TiAl alloy were successively replaced by silicon atoms, with their number increasing to six. Silicon was considered only on the Al sublattice (Fig. 1a), since the substitution of titanium by 1 eV is energetically less favorable. The calculated W_{sep} values are presented in Fig. 1b. It is evident that the increase in silicon concentration at the interface leads to a monotonic decrease in its strength (from 10.4 to 8.6 J/m^2, i.e. by $\sim$0.3 J/m^2 per Si atom). Analysis of the atomic structure of the interfaces showed that the length of the O–Si bonds is, on average, 0.25 Å longer than that of O–Al. Since the atomic radius of Si is 0.35 Å smaller than that of Al, this indicates a weakening of the interatomic interaction. In addition, the appearance of silicon in the interface layer of the TiAl alloy also leads to a slight increase in the interface distance by $\sim$0.02 Å per silicon atom. Analysis of the calculated local densities of electron states of interface atoms showed that an increase in the number of silicon atoms is reflected in the width of the low-lying peaks of both Si and O, and also leads to their splitting and the appearance of antibonding states (Fig. 2), which also indicates a weakening of the interface bonds and a decrease in W_{sep}.

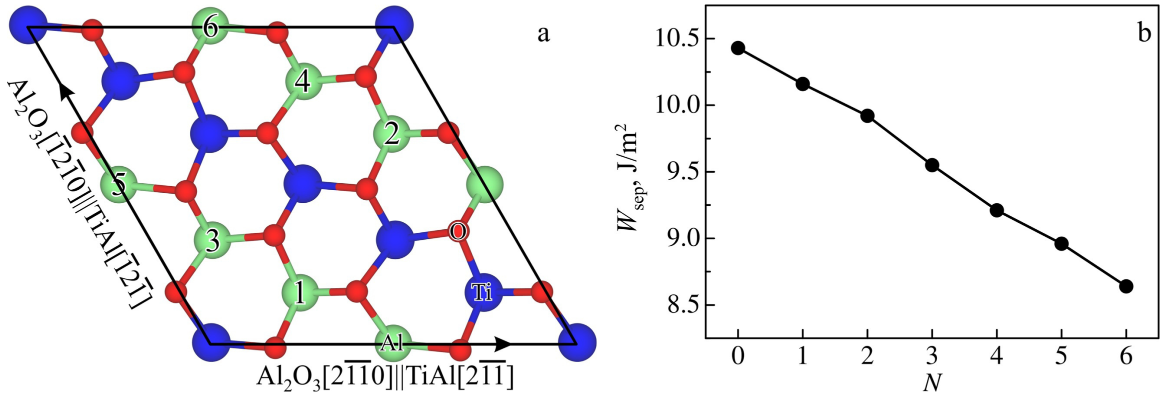

FIG. 1. Atomic structure of the interface layers of the γ-TiAl alloy and the α-Al_2O_3 oxide with indication of Si positions during sequential substitution of Al atoms (a), as well as adhesion energy at the α-Al_2O_3/γ-TiAl interface depending on the number of Si atoms (N) in the alloy interface layer (b)

An estimation of the segregation energy of silicon to the Al_2O_3/TiAl interface showed that this process is endothermic and requires more energy, the higher the silicon concentration at the interface. Thus, the segregation energy of the first silicon atom is 0.59 eV, the second – 0.62 eV, the sixth – 1.12 eV. Since silicon atoms are cations due to charge transfer to oxygen, the Coulomb repulsion between them causes an increase in the segregation energy. If the γ-TiAl alloy forms an interface with Ti_5Si_3, then Si segregation requires less energy.

According to experimental data [6], when a certain critical value of silicon concentration is exceeded, titanium silicide films, in particular Ti_5Si_3, begin to form. In order to estimate W_{sep} at both new interfaces the Al_2O_3(0001)-(3×3) surface cell with a parameter of 14.298 Å was aligned with the Ti_5Si_3(0001)-(2×2) cell, the parameter of which is 14.933 Å (Fig. 3a,b). Since Young's modulus of the oxide is 1.5 times greater than that of the silicide, the interface parameters corresponded to those of the oxide.

In the case of the Ti_5Si_3/TiAl interface the Ti_5Si_3(0001)-(2×2) surface cell was aligned with the TiAl(111)–($\sqrt{7} \times \sqrt{7}$) cell (Fig. 3c,d), the parameter of which is 14.688 Å. Since in this case Young's moduli of the silicide and the alloy are comparable ($\sim$230 GPa), the silicide film was compressed by 0.8% in the interface plane, and the alloy was stretched by the same value. Thus, the parameter of the interface cell was equal to 14.810 Å. Combinations of two silicide terminations (mixed and titanium) and one alloy termination were considered, since the alloy surface (111) has

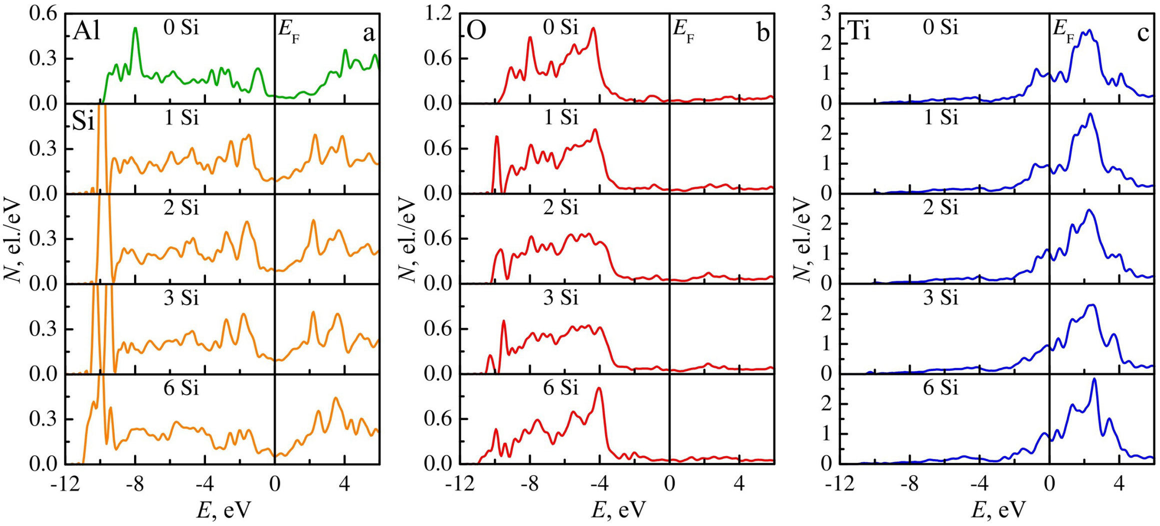

FIG. 2. Densities of electron states of the Al or Si atoms in the site 1 (see Fig. 1a) (a), as well as of the nearest O (b) and Ti (c) atoms

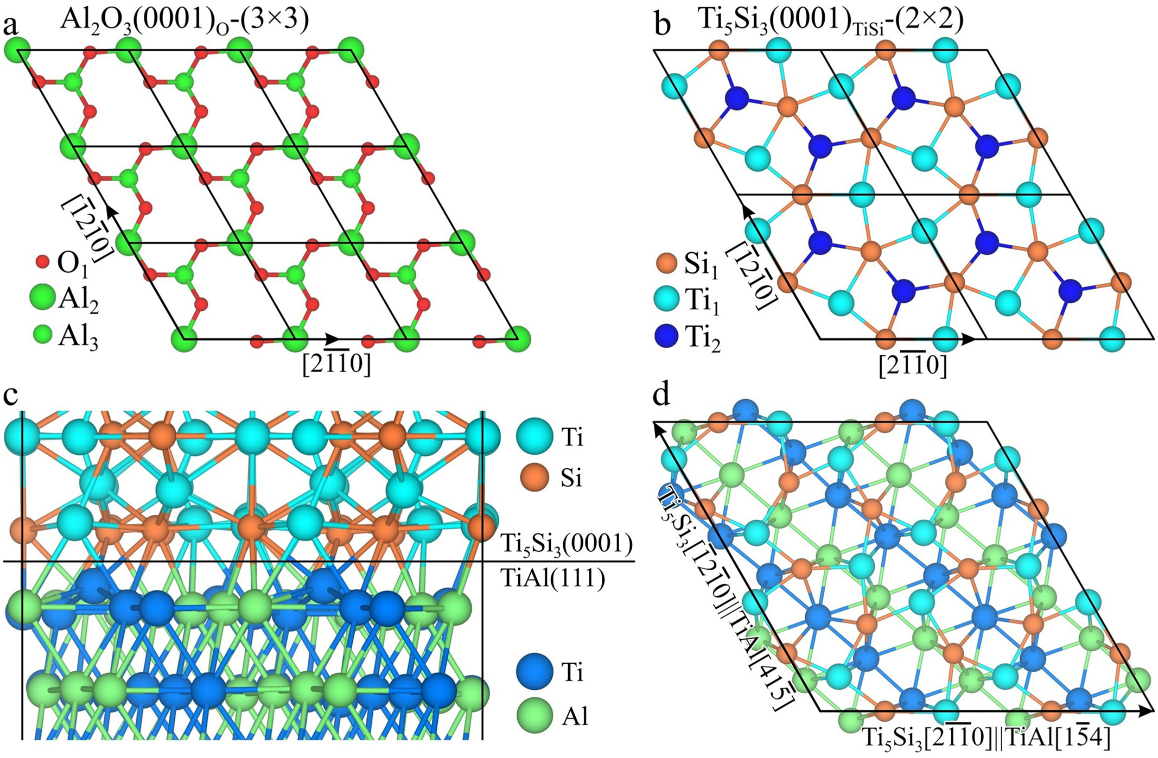

FIG. 3. Atomic structure of $Al_2O_3(0001)$-(3×3) (a) and $Ti_5Si_3(0001)$-(2×2) (b) surfaces, as well as of the $Ti_5Si_3(0001)$-(2×2)/TiAl(111)-($\sqrt{7} \times \sqrt{7}$) interface: side (c) and top (d) view

a stoichiometric composition. As the present calculations showed, the optimal number of atomic layers in the films was 5–7 layers for titanium silicide and 3–5 layers for the alloy. The number of atoms in the cell was 172 for the minimum film thicknesses.

As a result, the adhesion energy decreases at both interfaces (oxide–silicide–alloy) compared to the ideal interface, but at the Al_2O_3/Ti_5Si_3 interface, according to the present calculations, it remains quite high (7.9–8.3 J/m^2), whereas at the Ti_5Si_3/TiAl interface the W_{sep} values are equal to 2.26–2.80 J/m^2 depending on the contact configuration. Such a decrease in W_{sep} is explained by a change in the chemical bond mechanism from ionic-covalent for the oxide–alloy interface to metal-covalent (titanium silicide–alloy interface).

3.2. Oxygen diffusion through interface

To estimate the oxygen migration barriers, it is necessary to know the energies of the system with oxygen atoms in different interstitial positions in the interface layers and in the bulk. First of all, several interstitial positions of the oxygen atom in the alloy near the ideal interface TiAl(111)/$Al_2O_3(0001)_O$ were considered. Recall that in the bulk of the γ-TiAl alloy there are three interstitial positions: two octahedral (O1 and O2) with a local environment of Ti4Al2 and Ti2Al4, respectively, and a tetrahedral one – T (Ti2Al2). In the case of the alloy–oxide interface, the octahedral positions remain the same, and the tetrahedral positions can be divided into two types: T1 is a position in a tetrahedron formed by two Ti atoms and one Al atom of the interface layer and an Al atom of the layer second from the interface, and T2 is in a tetrahedron when the Al atoms are in the interface layer and the Ti atoms belong to different layers (Fig. 4a). The highest absorption energy (E_{abs}) when oxygen incorporates in the interface layers is 0.31 eV lower than in the γ-TiAl alloy and corresponds to the T1-position (3.93 eV). At the same time, E_{abs} of oxygen in the T2 and O1 positions is only slightly lower by 0.08 and 0.11 eV, whereas it reaches only 2.54 eV in the O_2 position (Fig. 4b). It should be noted that lower E_{abs} values indicate lower migration barriers from interface positions. The distribution of the charge density difference demonstrates ionic character of the O–Ti bonds, with Al atoms giving up a significantly smaller charge to O. In general, a correlation is observed between the absorption energies in the considered interstitial positions and the charge transfer to oxygen from the nearest atoms.

Substitution of some alloy Al atoms in the interface layers by Si leads to destabilization of some interstitial positions depending on the silicon concentration and its location relative to oxygen. Note that more than 30 configurations of O and Si atoms were calculated for each concentration of the latter. The highest absorption energy values depending on the number of silicon atoms are shown in Fig. 4b. It is evident that when oxygen is incorporated into the O1-position, the absorption energy decreases by $\sim$0.32 eV (in the case of two Si atoms), and then with an increase in their number, E_{abs} remains virtually unchanged. On the contrary, the absorption energy increases when oxygen occupies the O2 or T1 positions. However, in the presence of one or two silicon atoms, the O2 and T2 positions (not shown in Fig. 4b) are unstable, and oxygen shifts to the O1 and T1 positions, respectively. The change in the absorption energy in interstitial positions depending on the silicon concentration can be explained from the analysis of electronic and structural factors. If the third silicon atom is located in the first neighbors of oxygen in the T1-position, this leads to its instability, and the oxygen shifts to the O2-position, which in turn is unstable at a low Si concentration.

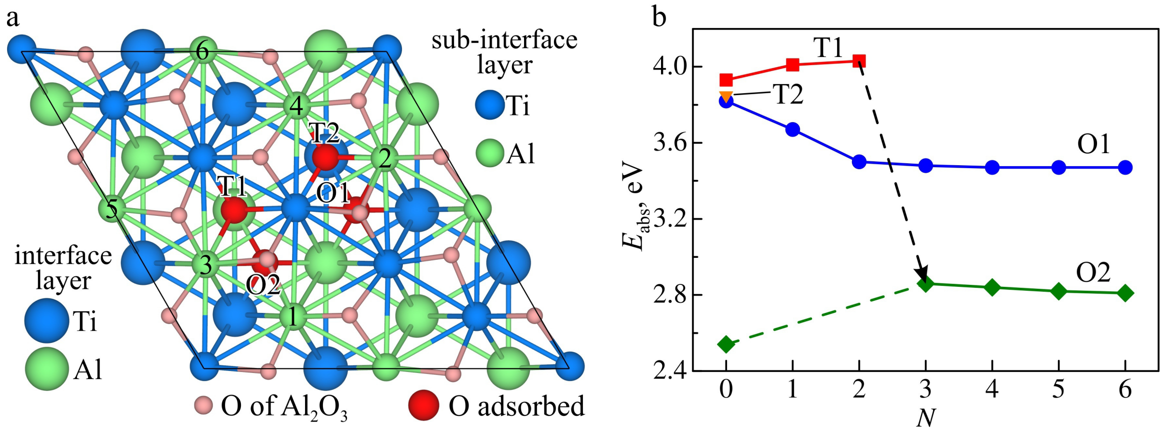

FIG. 4. Oxygen absorption positions in the Al_2O_3/TiAl interface layers with indication of Si positions during sequential substitution of Al atoms (a), as well as its absorption energy in these positions depending on the number of Si atoms (N) in the interface layer of the alloy

A few words should be said about the possible pathways of oxygen penetration from the oxide into the alloy. The present calculation of oxygen sorption on the (111) surface showed that the most preferred position is above the Ti2Al triangle of the surface layer, while the energy of oxygen sorption above the TiAl2 triangle is $\sim$1 eV lower. From the latter position, it is easier for oxygen to penetrate into the subsurface layers, since the oxygen binding energy in it is the lowest. The stable configuration of the TiAl(111)/$Al_2O_3(0001)_O$ interface suggests that oxygen atoms occupy both of these positions. It is easiest for oxygen from the oxide interface layer to penetrate into the O-positions in the alloy, since in this case the saddle point is located in the center of the Ti2Al triangle for O1 or TiAl2 for O2. Despite the fact that the O2-position is less preferred, in this case, as noted above, oxygen atoms require less energy to diffuse into it and continue further diffusion into the alloy. Calculations have shown that only in the first interface layers oxygen behaves somewhat differently from the bulk alloy. Subsequently, the tetrahedral positions become identical, and oxygen migration requires the same energies as in the bulk alloy [18]. Thus, the most energetically preferable path for oxygen penetration into the TiAl alloy goes through the O2→T→O2→T→O2→... positions (Fig. 5), and the Ti-rich O1-positions can serve as oxygen traps. With an increase in the silicon concentration in the alloy interface layer, the oxygen absorption energy in the O1-position decreases, as can be seen from Fig. 4b, but remains higher than in O2, so its introduction into the alloy interface layers will be preferable through the O2-position. Since silicon increases E_{abs} in the O2-position, it acts as an inhibitor, slowing down the oxygen penetration from the oxide into the alloy.

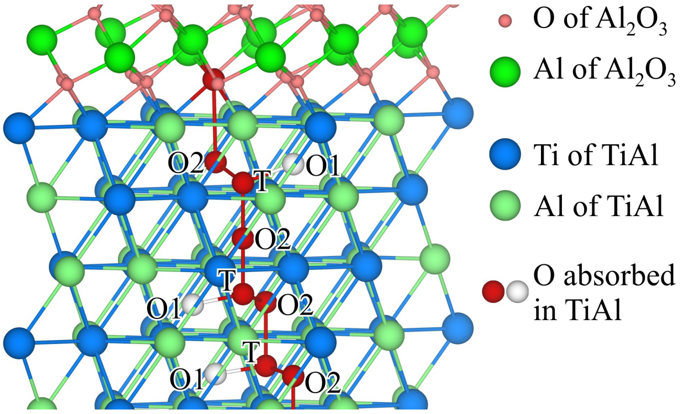

FIG. 5. The most preferred pathway for oxygen migration into the alloy

It is known that the average value of the diffusion coefficient in a system with an interface is estimated as the harmonic mean [19], and if the thicknesses of the contacting materials are different, then as the weighted harmonic mean. Thus, the effective diffusion coefficient of oxygen, which determines the rate of its penetration into the alloy to a certain depth, can be estimated by the formula:

$$D = \frac{l_{si} + l_{al}}{l_{si}/D_{si} + l_{al}/D_{al}}, \tag{1}$$

where the indices "*si*" and "*al*" refer to Ti_5Si_3 and TiAl; l_{si} is the thickness of the titanium silicide film, l_{al} is the depth of oxygen penetration into the alloy, and D_{si} and D_{al} are the diffusion coefficients of oxygen in the silicide and the alloy, respectively. The values of these coefficients were calculated using the Landman method [20] and within the framework of the statistical approach [21]. The results of the diffusion coefficient calculations were discussed in detail in [18, 22]. In general, the obtained values of the oxygen diffusion coefficient in titanium silicide are comparable with the values obtained for α-Al_2O_3 [23] and lower than for TiO_2 [24]. However, this coefficient was 9–14 orders of magnitude lower at a temperature of 1000–1700 K than in the TiAl alloy [18]. The oxygen diffusion coefficient in titanium silicide along the [0001] axis is $9.47\cdot10^{-7}\exp(-2.52/k_BT)$ m^2/s [22], and in the γ-TiAl alloy – $10^{-6}\exp(-1.25/k_BT)$ m^2/s [18]. This direction of diffusion in Ti_5Si_3 was chosen for two reasons: 1) the present model assumes that the silicide axis [0001] is oriented normal to the interface; 2) diffusion in this direction is the fastest.

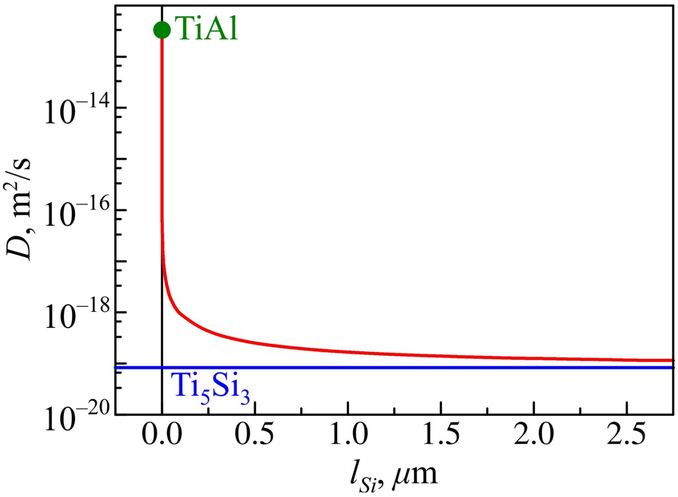

FIG. 6. Oxygen effective diffusion coefficient (red line) in the Ti_5Si_3/TiAl system as a function of the titanium silicide film thickness. The diffusion coefficients in the bulk alloy and titanium silicide are shown in green and blue, respectively

In addition, the study of oxygen adsorption on the $Ti_5Si_3(0001)$ surface showed that the most preferable position for oxygen is above the titanium triangles, and the introduction of oxygen into the subsurface layers will occur along the [0001] direction along the octahedral positions. Calculation of migration paths in titanium silicide confirmed the presence of a fast diffusion channel along this direction, while diffusion in the perpendicular direction is slower by several orders of magnitude. Thus, the present model allows us to lower-bound estimate the effect of the silicide film on oxygen diffusion. It is known that the thickness of the Ti_5Si_3 film can reach 3 μm [25]. It will be assumed that oxygen penetrates into the alloy to a depth of 1 μm at a temperature of 973 K.

The obtained dependence of the effective diffusion coefficient on the thickness of the titanium silicide film is shown in Fig. 6. The diffusion coefficients of oxygen in TiAl and Ti_5Si_3 are also given here. It is evident that even the formation of a thin Ti_5Si_3 film leads to a sharp decrease in oxygen diffusivity. Thus, it can be concluded that both silicon itself and the Ti_5Si_3 film actually contribute to slowing down oxygen diffusion in the γ-TiAl alloy, which is beneficial for increasing its corrosion resistance.

4. Conclusions

The adhesion energy of the doped by silicon α-Al_2O_3/γ-TiAl interface and that with the formation intermediate layers of Ti_5Si_3 was calculated. It was found that the substitution of aluminum by silicon leads to a decrease in the work of separation by $\sim$0.3 J/m^2 per Si atom, but its value remains high ($\sim$8.60 J/m^2) when all Al interface atoms are replaced by Si. When the Ti_5Si_3 film is formed, W_{sep} decreases to a lesser extent at the Al_2O_3/Ti_5Si_3 interface compared to the ideal Al_2O_3/TiAl one, whereas at the Ti_5Si_3/TiAl interface the work of separation is only 2.26–2.80 J/m^2, depending on the contact configuration. This is explained by a change in the chemical bonding mechanism from ionic-covalent to metal-covalent.

It is shown that the most energetically preferable way of oxygen penetration into the alloy is the path $O2 \to T \to O2 \to T \to O2 \to \ldots$, whereas the Ti-rich O1-positions can trap the oxygen atoms. In general, silicon acts as an inhibitor, slowing down the penetration of oxygen from the oxide into the alloy. Evaluation of the oxygen effective diffusion coefficient showed that the formation of a thin Ti_5Si_3 film leads to a sharp decrease in oxygen diffusivity. Thus, titanium silicide can serve as an effective diffusion barrier and prevent oxygen diffusion into the TiAl alloy, which is generally favorable for increasing its corrosion resistance.

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