Original Research Article

J. Funct. Mater. Biomol. 1(2)-2017 pp 51-53

SACRED HEART RESEARCH PUBLICATIONS

Journal of Functional Materials and Biomolecules

Journal homepage: www.shcpub.edu.in

ISSN: 2456-9429

Durability of grain interfaces in $TiAl_3$, TiAl, and Ti_3Al systems: A computer study

V. G. Zavodinsky* and Yu.G. Kabaldin

Received on 26 July 2017, Accepted on 03 Oct 2017

Abstract

Density functional theory and pseudopotentials were used to study reaction of the grain interfaces in the $TiAl_3$, TiAl, and Ti_3Al compounds on tensile deformations. It was shown that durability of the interfaces increases with increasing of partial amount of titanium while plasticity increases initially (from pure Al to $TiAl_3$) but then decreases.

Keywords: ab initio simulation, titanium aluminida, grain interfaces, tensile strength, plasticity

1 Introduction

Titanium-aluminum systems represent a great interest for the aerospace industry and for creation of sheetings [1, 2]. Important feature of Ti-Al systems is change of crystal structure at change of a ratio of the titan and aluminum contents. Besides, even for phases, identical in chemical composition, various isomorphisms are observed [3, 4]. The stable phases $TiAl_3$, TiAl and Ti_3Al are the most known [5, 6]. The crystal structures corresponding to them are described in [6]. These phases have similar mechanical properties. The most characteristic of them are high strength (from 1 GPa to 2.5 GPa) and high malleability. Depending on technology durability and plasticity of systems can increase or decrease with increase of the content of aluminum. In the work [7] it is noted that they possess the low plasticity: their relative breaking lengthening does not exceed 1-2 percent. However data on relative lengthening of 5-10 percent are provided in work [8]. Moreover, in recent time there were data that Ti-Al systems can possess the superplasticity [9] under certain conditions.

It seems useful to investigate the systems TiAl3, TiAl and Ti3Al in identical conditions, in lack of dislocations, doubles and other collective effects; in other words, to consider idealized model systems in which durability of material is defined only by durability of grain interfaces. Perhaps, results of such research will help to answer a question: how the ratio of the aluminum and titan amounts influences durability and plasticity of their compounds?

Our work is devoted to quantum-mechanical study of durability of grain interfaces in the $TiAl_3$, TiAl, and Ti_3Al systems.

2 Methods and models

For studying of the Ti_3Al system we took structure of cubic type (space group Pm3m) with the lattice constant of 0.4109 nm. For the TiAl system the structure with the tetragonal crystal lattice (P4/mmm group) with parameters a= 0.3988 nm and c= 0.4079 nm is used. For the $TiAl_3$ compound the bulk centered tetragonal lattice (P4/mmm group) with parameters a= 0.5446 nm, c = 0.8608 nm is taken [4]. Pure aluminum possesses a face-centered lattice with parameter a=0.4040 nm.

An interface between two grains was modeled as a contact of two thin crystalline slabs having infinity dimensions in X and Y directions and a nanoscale thickness in Z direction. Durability of the grain interface was found by gradual increasing in distance between outer sides of slabs up to a rupture of contact between them. For comparison we considered also border of grains in pure aluminum and in the aluminum which is poorly alloyed by titanium. Schemes of contacts are presented in Figure 1.

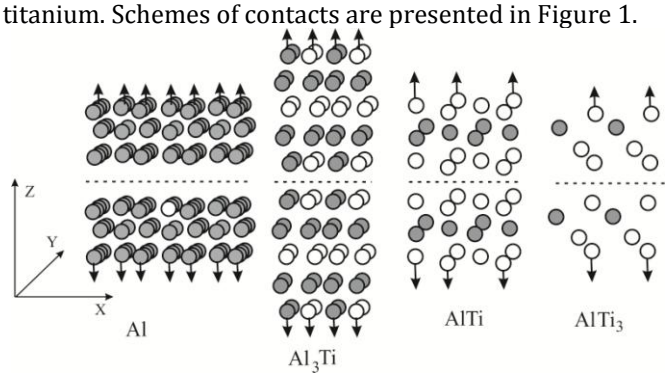

Figure 1. Schemes of our modeling grain interfaces in aluminum and in titanium alyuminida. Wight circles present Ti atoms; gray circles show Al atoms.

In this work we used the FHI96md package [10] realized within based on the density functional theory (DFT) [11, 12] and the pseudopotential method [13]. This package was previously used with advantage for many systems, including transition metal compositions [14-16].

In all cases, the generalized gradient approximation

* Corresponding author e-mail: vzavod@mail.ru
Phone: +07962 583 1543, Fax: +074212 226 589
Institute for Materials Science, 153 Tikhookeanskaya str., Khabarovsk, 680042, Russia

[17] to description of the exchange-correlation interactions has been chosen and the optimization of the atomic geometry has been performed. All pseudopotentials were constructed with the FHI98PP package [18]. They were checked for the absent of the so-called 'ghost' states. The energy cutoff for the plane wave set was equal to 40 Ry.

We applied the following technique to research of durability of grain borders. The interacting slabs approached among themselves before the minimum of their total energy was achieved. After that the top and lower atoms of the system (marked in Figure 1 with shooters) were step by step displaced in the direction of *Z*, and fixed on each step. Other atoms of system had opportunity to be displaced under the influence of interatomic forces, and there was equilibrium again in the system. Thus, the distance between outer sides of the slabs increased, the intergrain border extended, and the total energy of the system changed.

We found the variations of the total energy ΔE as functions of elongation ΔZ, and then the applied strength P was calculated according the formula $P=\frac{\Delta E}{\Delta Z}\frac{1}{S_{XY}}$, where $\mathbf{S}_{XY}$ is the system square in the XY plane.

plied strength P was calculated according the formulae $P=\frac{\Delta E}{\Delta Z}\frac{1}{S_{XY}}$, where S_{XY} is the system square in the XY plane. In the shift case we studied the dependence of ΔE on

tgφ, where φ is the shift angle, and calculated the shift module G: $G=\frac{\Delta E}{\Delta X}\frac{1}{S_{XY}}\frac{1}{tg\,\phi}$.

3 Results and Discussion

First of all, we investigated durability of border of grains in pure aluminum. The result is presented in Figure 2 (curve Al).

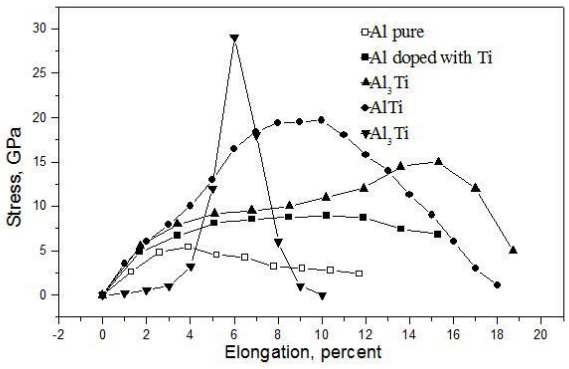

Figure 2. Dependence of stress on elongation of grain borders.

We see that the tensile strength of pure aluminum is close to 5.5 GPa, and the critical length of stretching with which destruction of border comes, is equal to 4 percent. The tensile strength received by us over exceeds many times the values observed at real aluminum materials. It no wonder as in real material there is a set of the factors reducing durability. Besides, the nano-scale size of the studied system also gives the contribution to increase of durability. The similar results were obtained in the work [18] for tungsten carbide nanoparticles.

Then we investigated influence of single atom of Ti placed on the border between aluminum grains; results are presented in Figure 2 too. These calculations simulate aluminum lightly alloyed with titanium: one atom of Ti is the share of 45 atoms of Al. We see that Ti as an impurity increases strength of aluminum approximately by one and a half times, and plasticity increases approximately twice.

Further we carried out similar calculations for compounds $TiAl_3$, TiAl, and Ti_3Al. In the first case one atom of Ti is the share of three atoms of Al; in the second case the contents of Al and Ti are identical; in the third case three atoms of Ti fall on one atom of aluminum. In Table 1 data on values of strength and of relative lengthening limit for all studied systems are collected.

Table 1. Values of tensile strength *P* and the limit of lengthening *L* for studied systems.

System	*P*, GPa	*L*, percent
Pure Al	5.5	4
Al doped with Ti	9.0	9
Al_3Ti	15.0	15
AlTi	20.0	10
$AlTi_3$	29.0	6

We see that at increasing of the relative content of Ti (from 1/45 to 1/3) both the tensile strength and the relative lengthening limit considerably increase. When amounts of titanium and aluminum becomes identical the tensile strength still increases, while plasticity decreases. The further increase in the relative content of Ti (from 1/1 to 3/1) leads to even bigger growth of the tensile strength and to sharp reduction of plasticity.

Thus, we see that in systems where there are no dislocations and other defects influencing mobility of atoms and atomic complexes, durability of material determined by durability of grain borders, is higher in those systems in which the content of aluminum is less than the content of titanium. Plasticity behaves no monotonously. At small amounts of Ti (up to 1/3) its presence increases plasticity, and at large contents (1/1 – 3/1) plasticity decreases.

4 Conclusions

Results of quantum modeling testify that in the absence of additional factors (like dislocations, twins and so forth) durability of intermetallida grows with increase in content of titanium; plasticity grows in the beginning, and then decreases, keeping its value in the interval of 10-15 percent.

Acknowledgements

This work is supported by grants of the Russian Research Foundation "Development of program and hardware for the system of intellectual diagnostics of vehicles and constructions in the Arctic conditions at the remote access".

References

[1] V.I. Ivanov, K.K.Yasinskiy. Tekhnologiya legkikh splavov. 3, (1996) 20-23 (in Russian).
[2] R.M.Imaev, V.M.Imaev, T.G.Khismatullin, M.Oehring, and F.Appel. Phys. Met. Metallography 102, (2006) 105–113.
[3] M.Asta, D.deFontaine, M.vanSchilfgaarde, M.Sluiter, and M.Methfessel. Phys. Rev. B 46 (1992) 5055-5072.
[4] A.A.Klopotov, M.G.Dementieva, A.I.Dolidchik, N.O.Solonitsyna, and E.V. Kozlov. Fundamental'nye problemy sovremennogo materialovedeniya 1, (2006) 112-120 (in Russian).
[5] E.H.Padilla, A.M.Villafañe, R.P.T.Soto, G.V.Olvera. J.G.Ch.Nava, L.B.Gómez, R.G.B.Margulis, and A.H.Macías. Int. J. Sci. Adv. Technol. 5(8), (2015) 1-6.
[6] M.Peters, C.Leyens. Titanium and titanium alloys: fundamentals and applications. (Wiley: VCH Verlag, 2003. 532 p.)
[7] B.A.Kolachev, A.A.Il'in, and P.D.Drozdov. Metally. 3, (2001) 41–48 (in Russian).
[8] N.Podrezov, I.D. Gornaya, M.V. Remez, B.S. Goltvyanitsa, S.K. Goltvyanitsa. www.materials.kiev.ua/publications/EMMM/2012/8.pdf (in Russian).
[9] R.M.Imaev, V.M.Imaev. Lett. Mater. 5(3), (2015) 253-257.
[10] M.Beckstedte, A.Kley, J.Neugebauer, and M.Scheffler. Comp. Phys. Commun. 107, (1997) 187-205.
[11] H.Hohenberg, W.Kohn. Phys. Rev. 136, (1964) B864-71.
[12] W.Kohn, J.L.Sham. Phys. Rev. 140 (1965) A1133-38.
[13] M.L.Cohen, V.Heine. In: Solid State Physics, V. 24. Ehrenreich H, Seitz F, Turnbull D, editors. (Academic Press; New York, 1970), 38-249.
[14] J.Dabrowski, H.-J.Mussig, V.G.Zavodinsky, R.Baierle, and M.J.Caldas. Phys. Rev. B 65 (2002); 245-305.
[15] V.G.Zavodinsky. Phys. Solid State 46(3), (2004) 453-457.
[16] Zavodinsky VG. Int. J. Refr. Met. Hard Mater. 28, (2010) 446-450.
[17] J.P.Perdew, K.Burke, and Y.Wang. Phys. Rev. B 54, (1996) 16533-16539.
[18] M.Fuchs, M. Scheffle. Comp. Phys. Commun. 119, (1999). 67-165.