



# Preparation of TiAl–Cr surface alloy by plasma-surface alloying technique

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## ABSTRACT

A plasma-surface technique was used to form a TiAl–Cr alloy on the surface of a TiAl-based alloy. The feasibility of the alloying process was evaluated by a first principle calculation method. The preparation process was optimized by investigating the effects of processing temperature and discharge pressure on the formation of surface alloy. The calculation using the first-principle method showed that the addition of Cr into the TiAl lattice would increase the stability of the system, and improve mechanical properties of the alloy. The processing temperature was selected at 1100 °C, slightly below the eutectic temperature of the Ti–Al system, ensuring diffusion efficiency and also avoiding the degradation of substrate microstructure. The optimum discharge pressure was 25 Pa within the range of 12–55 Pa. Sputtering and diffusion were well coordinated at this pressure and the obtained alloyed layer had the largest thickness.

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## 1. Introduction

TiAl based alloy is an attractive structural material for the aero-industry, due to its high specific strength. However, there still exist major obstacles which restrain introducing TiAl-based alloy to aero-engines, especially the insufficient oxidation resistance at high temperature and wear resistance of this alloy [1–3]. Enhancing oxidation and wear resistance of TiAl based alloy with surface engineering processes has long been a focus of intensive research. Protective coatings are the most frequently studied and applied methods, but they are often challenged by the interface problem or the compatibility of the modification layer with the substrate [4–8]. The aero-engine parts are usually working within demanding circumstances, synergism of vibration, thermal cycling, oxidation and wear are inevitable, therefore the weakness of an interface is fatal for the safety and lifetime of the machine. The Plasma surface alloying process is a new approach of surface engineering, as its modification layer is a diffusion layer metallurgically bonded with the substrate, without the concern of an interface problem. Previous studies on surface alloying of titanium alloy and TiAl-based alloys have shown that the process is an effective way of preparing various diffusion layers with improved properties compared with the untreated original materials, such as wear-resistance and oxidation-resistance [9–12]. The composition and thickness of the alloyed layer can be controlled by adjusting the processing parameters. In this study, the plasma surface

chromizing process was conducted on TiAl-based alloy, as it has been generally acknowledged that the addition of Cr into TiAl-based alloy is beneficial to improve its oxidation resistance [13,14]. The feasibility of the alloying process was evaluated by observing the impact of Cr addition on the thermodynamic stability of the system through a first principle calculation. In addition, the processing condition was optimized by investigating the influence of treating temperature and discharge pressure on the formation of the alloyed layer.

## 2. Experimental

The first principle calculation was based on the CASTEP module of Materials Studio with local density approximation method. The periodic crystal model of the object was set up and optimized. The changes of formation and binding energy were calculated considering the probable lattice position that the added Cr atom would occupy.

The principle of the plasma surface alloying process is illustrated in Fig. 1. Within the vacuum glow discharge chamber, the sputtering target and the substrate are the cathodes of glow discharge and connected to two independent power suppliers. The sputtering target is made of pure chromium, the substrate is the TiAl-based alloy sample. As the vacuum is established, argon is admitted at the appropriate gas pressure. Turning on the power suppliers, the glow discharge is initiated. The chromium atoms are sputtered from the target and deposited on surface of the sample which is heated by ion bombardment to high temperature, thereafter, the alloyed layer is formed through thermal diffusion process.

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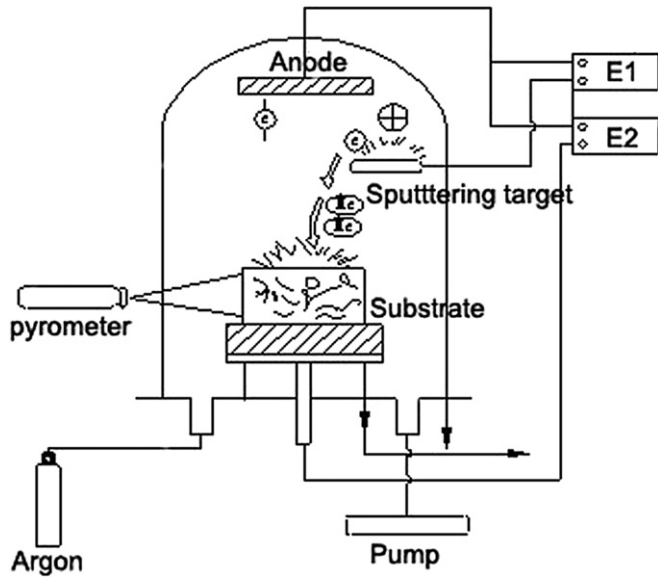


Fig. 1. The sketch of set up of the plasma surface alloying process.

**Table 1**  
The experimental parameters.

Experiment	Temperature (°C)	Pressure (Pa)	Processing time (h)
1	1000	25	4
2	1050	25	4
3	1100	25	4
4	1100	12	4
5	1100	25	4
6	1100	40	4
7	1100	55	4

Casting TiAl alloy with nominal composition Ti–46.5Al–2.5V–1.0Cr (at %) was used as substrate material. The samples were cut into squares dimensioned  $13 \times 13 \times 4$  mm, then polished to an average roughness of  $R_a < 0.05 \mu\text{m}$  and rinsed in acetone prior to the alloying treatment. The sputtering target was pure chromium (99.99 wt%) sheet dimensioned  $50 \times 50 \times 5$  mm. Pure argon (99.99%) was used as the discharge media.

The alloying treatment temperature was selected at the range of 1000–1100 °C to observe the alloying efficiency and the impact on substrate microstructure. Discharge pressure was also examined

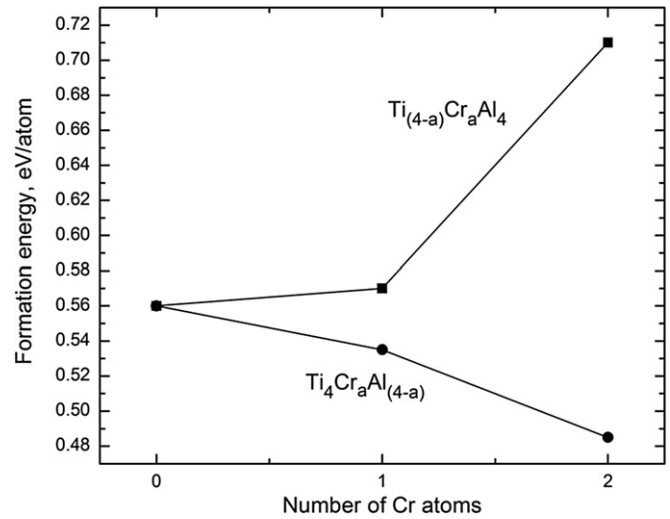


Fig. 3. The effect of Cr content on formation energy.

within range of 12–55 Pa to see the difference in thickness of the alloyed layer. In all the experiments, the processing time was 4 h, and other discharge-related parameters were fixed as follows: the sputtering voltage 800 V, substrate bias 350–400 V, target/substrate distance 18 mm. Table 1 shows the experimental parameters. An optical microscope was used to observe the cross-section microstructure of the alloyed layer. GDOES (Glow Discharge Optical Emission Spectroscopy GDA750) and microhardness tester (Leco M-400 H1) were used to analyse the composition profile and microhardness of the alloyed layer.

### 3. Results and discussion

#### 3.1. The calculation results of the first principle method

Supercell models were set up on the basis of the L10 unitcell of TiAl-based alloy. As solute atom, the possible lattice position that the adding Cr atom would take was either the position of the Ti atom or the position of the Al atom. Therefore the solid solution could be presented as  $\text{Ti}_{(4-a)}\text{Cr}_a\text{Al}_4$  or  $\text{Ti}_4\text{Cr}_a\text{Al}_{(4-a)}$ , and two of the examples are also given in Fig. 2, wherein one Cr atom was added into the supercell.

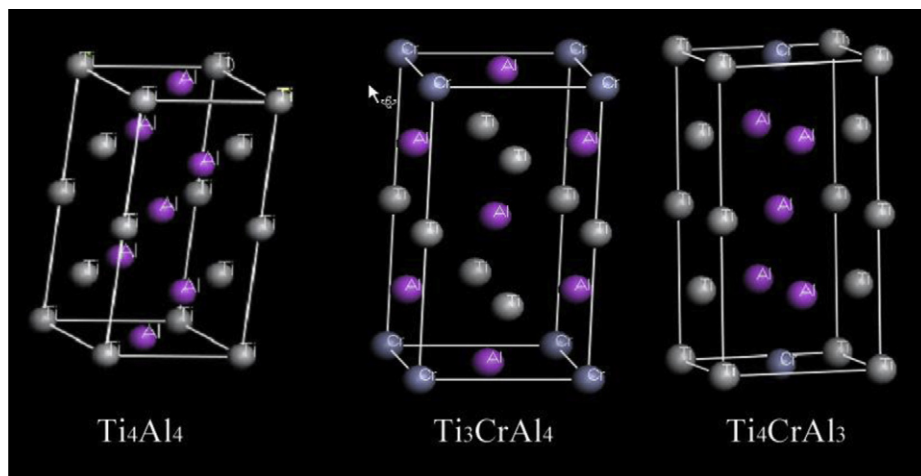


Fig. 2. The supercell models of TiAl with Cr addition.

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