

# Modelling of defects and amorphisation by ball milling of $\gamma$ -TiAl

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## Abstract

The formation and site preference energies and volume changes of single and pair of defects of ternary alloying elements in  $\gamma$ -TiAl intermetallic compound were studied by the density functional theory. Slight tendency to clusterization of antisite defects has been found. This may lead to disorder in the system. The V and Cr atoms prefer to reside in the Ti sublattice. The formation energy for Cr–Cr, Cr–V and V–V nearest neighbour pairs are in the 1.3–2 eV range. The Al antisite in Ti sublattice requires much less energy than the Ti antisite in Al sublattice. The amorphisation process of TiAl alloy was studied by means of high energy ball milling of Ti and Al elemental powders, which produces amorphous structure after 40 h. The amorphous states were studied by the DFT calculations of many random atomic configurations and the results were compared with the NiAl compound. Possible explanation for the amorphisation of the TiAl compound is presented.

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## 1. Introduction

Several ordered intermetallic alloys, such as NiAl and TiAl with other alloying additions, are currently being studied as light weight materials for high temperature applications [1–9].  $\gamma$ -TiAl (tetragonal  $L1_0$  structure) is one of the most promising compounds because of a good balance between density, strength and oxidation resistance, but it suffers from brittleness at low temperatures.

One of the possible methods for improving low temperature ductility is decrease of grain size by powder metallurgy starting with ball milling [1–3]. Ball milled samples show substantial grain refinement leading even to the amorphous structure after prolonged milling times [1–5,10–12]. Small additions of other elements like V or Nb catalyse formation of the amorphous structure at compositions near TiAl [5,6]. Contrary to TiAl, ball milling of powders of compositions near NiAl never results in the amorphous structure [7–9]. It results in the

nanocrystalline phase of B2 structure. The additions of up to 6 at.% of Fe, Ga, Mo, Co or Ti [8,9] do not change final B2 nanocrystalline structure.

These materials were also studied by various theoretical methods[14–19]. In this work we aim to extend these previous studies and to investigate the issue of the amorphisation of the TiAl compound.

We will first present an experimental structural study of TiAl and NiAl after ball milling and demonstrate experimental evidence for much better amorphisation of the TiAl alloy, as compared to NiAl. Then we will report on ab initio calculations of various aspects of this system having possible influence on the process of formation of the TiAl alloy. We will show the results for the formation and site preference energies, volume changes caused by Cr, V atomic impurities and antisite defects in TiAl. We will close the paper with the ab initio study of amorphisation process in this system.

## 2. Experimental procedure

Powders of titanium (110  $\mu\text{m}$  size and purity >99.5%), aluminium (150  $\mu\text{m}$  size and purity >99.5%) and nickel

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(100  $\mu\text{m}$  size and purity  $>99.5\%$ ) were used as starting materials. The powders were initially blended to the desired composition of 50Ti–50Al, 52Ti–48Al and 50Ni–50Al (at.%) under argon atmosphere in the glove box equipment. The mechanical alloying was carried out at room temperature in a planetary mill (Fritsch Pulverisette P5/4) at a rotation speed of 200 rpm and milling times up to 60 h. X-ray diffraction with Mo  $K\alpha$  radiation was used for structure examination with Philips PW 1830 diffractometer.

### 3. Experimental results

The high energy milling of 50Ni–50Al elemental powders resulted in the formation of ordered B2 nanocrystalline structure after 60 h. The structure has been obtained from the indexing of the peaks in the X-ray diffraction pattern (Fig. 1). Other situation has been observed for high energy milling of 50Ti–50Al alloy where only two diffuse peaks are found in the X-ray diffraction pattern (Fig. 2), it indicates that the sample is in the fully amorphous state. The sequence of phase transitions was observed during milling of elemental powder of the 52Ti–48Al composition alloy for up to 80 h (Fig. 3). The formation of TiAl solid solution manifested itself by disappearance of aluminium reflections and change of position of titanium reflections. It is observed already after 5 h of milling. Further milling causes total dissolution of aluminium in titanium (after 40 h of milling), resulting in a nanocrystalline TiAl solid solution. Finally, the transformation of supersaturated nanocrystalline TiAl solid solution into the amorphous phase occurs after 80 h.

### 4. Calculation method

The present ab initio calculations have been performed with VASP program [20,21] and PAW pseudopotentials [22]. The  $\gamma$ -TiAl alloy crystallises in tetragonal structure, space group  $P4/mmm$  ( $Z=1$ ). The Ti and Al atoms are located at  $(1/2, 1/2, 1/2)$  and  $(0, 0, 0)$ , respectively. Calculations of defect configurations were carried out within  $2 \times 2 \times 2$  supercell, subject to periodic boundary conditions and consisting of 16 atoms. For wave vector summation the  $6 \times 6 \times 6$

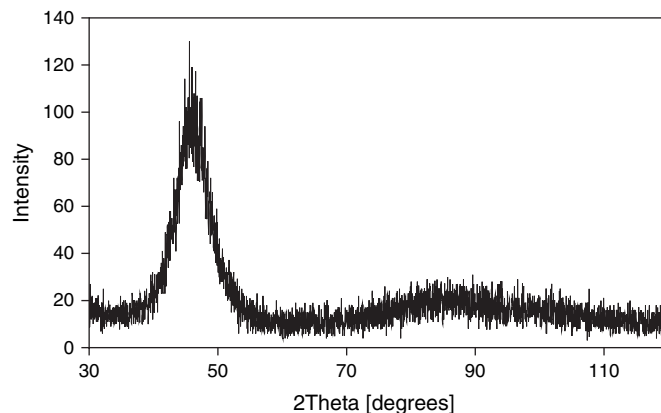


Fig. 2. X-ray diffraction pattern of 50Ti–50Al alloy milled for 60 h.

$k$ -mesh was used. All calculations for the simulated amorphous states were performed using the same calculation setup with respect to  $k$ -mesh and pseudopotentials used.

In the case of the crystalline material the main outcome of the optimisation of  $2 \times 2 \times 2$  supercell is the ground state energy denoted as  $E(A, B)$ , where  $A$  and  $B$  represent composition of the supercell in Ti and Al sublattices, respectively. For example,  $E(7\text{TiAl}, 8\text{Al})$  and  $E(7\text{TiCr}, 7\text{AlV})$  are the ground state energies of TiAl supercell with the additional Al in the Ti sublattice, and Cr in Ti and V in Al sublattices at the nearest neighbour distance, respectively.

Single defect, like impurity atom or antisite atom was located at the centre  $(1/2, 1/2, 1/2)$  of the  $2 \times 2 \times 2$  tetragonal supercell. This site and the atomic positions at  $(0, 0, 0)$ ,  $(1/2, 0, 0)$ ,  $(1/2, 1/2, 0)$ , and equivalent are fixed by symmetry. Atomic position close to  $(1/4, 1/4, 1/4)$  site was relaxed. The lattice parameters were kept constant at the values for the pure  $\gamma$ -TiAl crystal, which resulted in usually negative pressure. Such conditions are closer to real alloys with small concentration of defects, where the undisturbed lattice around the defect suppresses the relaxation of the size of the unit cell containing the defect.

In a double defect case (e.g. the pair Cr–V), two impurity atoms were placed as nearest neighbours. The atomic positions were relaxed, but the shape and lattice constants of the supercell were kept constant.

### 5. Results

The experimental lattice constants [23] of tetragonal ( $Z=1$ ) TiAl at room temperature  $a=2.829 \text{ \AA}$  and  $c=4.071 \text{ \AA}$  agree very well with our calculation which reads  $a=2.8134 \text{ \AA}$  and  $c=4.0736 \text{ \AA}$ . Table 1 gives the calculated ground state energies and external pressures of the  $2 \times 2 \times 2$  supercell with and without defects. The baseline pressure for the undisturbed crystal geometry used in calculation was  $P=4.1 \text{ kbar}$ . As seen from Table 1 the single defect and a pair of defects would generally decrease the volume of the supercell, since the residual pressure is negative. Only a Ti antisite atom or pair of antisite atoms would require to increase slightly the unit cell volume. In single defect calculations the

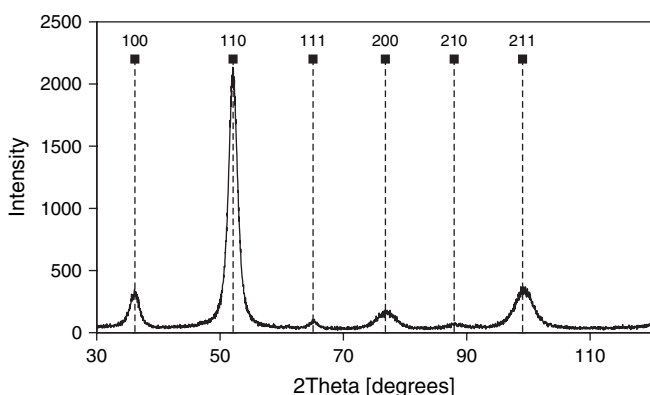


Fig. 1. X-ray diffraction pattern of 50Ni–50Al alloy milled for 60 h.

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