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Molecular-dynamics simulation of the synthesis of intermetallic Ti–Al

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ABSTRACT

In the present paper, results of a molecular-dynamics simulation study of the synthesis of intermetallic Ti–Al in the regime of thermal explosion at constant volume are reported. The structure of the polycrystalline intermetallic compound formed upon cooling was studied, and the dependence of crystallite sizes on the cooling rate was examined.

1. Introduction

An important problem in materials science is the synthesis of refractory materials with a high resistance to fracture. Among such materials are intermetallides, chemical compounds of metals featuring a complex crystal structure involving in some cases up to 30% covalent bonds. Such materials possess quite unusual physico-mechanical properties. For instance, alloys of the titanium/aluminum system exhibit many useful properties, such as good strength characteristics (168-GPa modulus of elasticity) [1] in combination with a low density (3.95×10^3 kg/m^3), a high resistance to heat (TiAl gas-turbine blades withstand temperatures up to 1100 K), and susceptibility to passivation [2]. Due to those properties, such alloys have found widespread use in aerospace, chemical, and petrochemical industries.

There are several methods to synthesize intermetallides; those methods can be classed either to quasi-static or dynamic methods. The most routinely used quasi-static methods are the self-propagating high-temperature synthesis (SHS) [3], the electrical-discharge powder consolidation technique [4], and the synthesis of intermetallics in the regime of thermal explosion [5]. To dynamic methods, shock compression of powders can be classed [6]. In recent years, intermetallic formation processes proceeding during gas-dynamic spraying of metals [7], during condensation of materials from plasma flows [8], and during electron-beam-induced synthesis of intermetallic materials [9] have been studied rather extensively, but, for the most part, just experimentally.

A most suitable method for theoretical treatment of intermetallic synthesis reactions is the molecular-dynamics method [10–13]. To date, many studies where the molecular-dynamics method was employed to numerically model the synthesis of intermetallides Ni–Al [14–21], Cu–Al [22], Ti–Al have been reported [23,24]. As the boundary conditions in [14–24], either periodicity conditions [18] or the condition of free boundary [14–17,19–24] were adopted. An analysis of the simulated data of [14–21] points to a substantial impact of boundary conditions on the kinetics of intermetallide synthesis reactions.

Weingarten and Rice examined synthesis of intermetallic NiAl at a constant pressure generated at the interface between two planar Ni and Al plates [18]. The calculations were performed using the molecular-dynamics method for NPT ensemble and periodic boundary conditions over all directions. The suitability of periodic boundary conditions was only justified for a periodic system formed by an infinite number of alternating Ni and Al layers. In the case of two plates, the use of periodic boundary conditions results in the occurrence, in simulations, of non-physical transport effects for Al atoms. The atomic configurations of reacting Ni and Al plates at two times are shown in Fig. 4 (c),(d) of paper [18]. Evidently, some Al atoms initially contained in the lower plate entered the upper Ni plate due to the periodic boundary conditions used (not via diffusion). In the course of simulations, Al atoms left the

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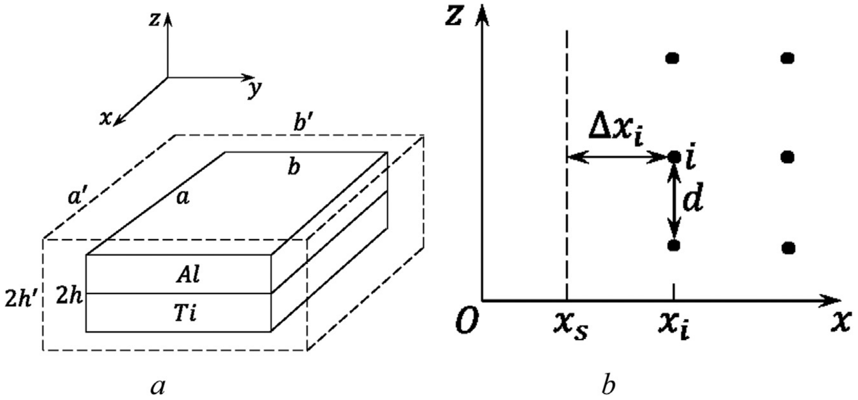

Fig. 1. (a). The Ti and Al plates contained in a rectangular box (shown with dashed lines); (b). The flat wall of the box ($x_s = \text{const}$) normal to the axis x and the distribution of atoms in the vicinity of the wall ($\Delta x_i = x_i - x_s = 1\text{Å}$ is the separation between the boundary i-atoms and the wall, and d is the equilibrium interatomic separation).

calculation domain through the lower boundary, and they entered, through the upper boundary, the upper plate formed by Ni atoms. As a result, Al atoms were instantaneously transported to the upper boundary of the Ni plate, and they then diffused into that plate.

All other authors considered the same problem as stated in spherical geometry [14–24]. Prior to the beginning of the alloying reaction, a spherical nanoparticle formed by atoms «A» was covered with a spherical layer of finite thickness formed by atoms «B». On heating, diffusion of atoms «A» and «B» across the internal interface occurred while the outer boundary of the layer occupied by atoms «B» was a free boundary. As it was shown in [24], in the latter case the kinetics of the reaction largely depends on the modification of the boundary-layer atomic structure. Consider in now more detail the results obtained in [23,24].

In [23,24], the molecular-dynamics method was used to examine, with the help of an embedded-atom method (EAM) potential [13], the synthesis of intermetallic γ-TiAl. In [23], initially an Al nanoparticle at temperature $T_0 = 100$ K covered with a Ti monoatomic layer, was specified. Then, the nanoparticle was uniformly heated to temperature $T_{\max} = 1700$ K. At $T_R = 1352$ K, an alloying reaction of Ti and Al was initiated at constant pressure $P \approx 0$. Then, the obtained intermetallic γ-TiAl was cooled to a finite temperature ($T = 100$ K). An analysis of the atomistic structure thus formed has showed that, in its final state, the intermetallic γ-TiAl tended to develop an amorphous short-range icosahedral structure [12]. The obtained stable structure was considered in [23] as a metastable state of supercooled liquid. As it was noted in [23], the non-occurrence of crystallization in melted γ-TiAl was rather a strange result. However, in publications [15–17] by the same authors, where a similar simulation study of the formation process of intermetallic NiAl was reported, possible occurrence of crystallization during cooling of the intermetallic has been demonstrated. In our opinion, the former paradoxical finding could be a result of possible absence of nucleation centers in the γ-TiAl melt.

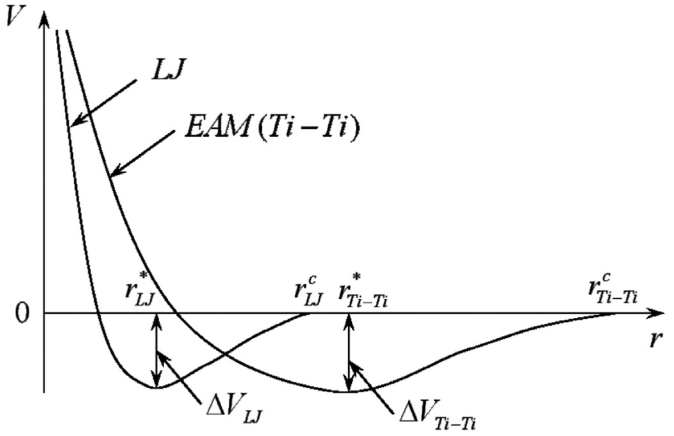

Fig. 2. The interaction potential V versus distance r: EAM (Ti–Ti) – effective potential of Ti–Ti interaction [13], $\Delta V_{\text{Ti-Ti}}$ – depth of potential well at equilibrium separation $r^*_{\text{Ti-Ti}}$ between atoms, $r^c_{\text{Ti-Ti}}$ – cutoff radius; LJ–Lennard–Jones potential for the interaction of boundary atoms with the wall, ΔV_{LJ} – depth of potential well at equilibrium separation r^*_{LJ} between atoms, r^c_{LJ} – cutoff radius.

In the case of a spherical particle, the kinetics of the reaction proved to be influenced by particle surface curvature. Levchenko et al. showed that the reaction proceeded much less rapidly when a Ti particle was covered with an Al layer in comparison with the case in which an Al particle coated with Ti was considered [24]. That phenomenon can be attributed to the action of elastic stresses, whose magnitude varied in proportion to the radius of curvature. Under such stresses, plastic deformation developed in the Al layer, and this deformation then initiated a pre-alloying process at the interface between Ti and Al [24]. The layer formed as a result of the reaction acted as a barrier for the synthesis of intermetallic TiAl. Thus, the above analysis of publications [14–24] shows that, in modeling the synthesis of intermetallic «AB» one may encounter serious difficulties in posing boundary conditions of periodic or free-boundary type.

2. Statement of the problem

2.1. Physical statement of the simulation problem for synthesis of an intermetallic at constant volume

In the present study, we modeled synthesis of intermetallic γ-TiAl conducted under conditions close to the conditions adopted in the experiment of [25], where intermetallic TiAl_3 was synthesized at constant volume in the regime of thermal explosion. The problem was treated by the molecular-dynamics method using the interaction potential reported in [13]. The case of two plates, a Ti plate and an Al plate, was considered. The upper plate was formed by 6844 (53%) Al atoms (fcc lattice), and the lower plate comprised 5967 (47%) Ti atoms forming an α-Ti material (hcp lattice). Both plates had identical dimensions $a \times b \times h = 80 \times 80 \times 20$ Å, with their ribs a, b, and h being directed respectively along the axes x, y, and z (Fig. 1 (a)). Both plates, Ti and Al, were placed in a rectangular box with sizes $a' \times b' \times 2h' = 82 \times 82 \times 42$ Å. The interaction of Ti and Al atoms with the walls was modeled with the help of a Lennard–Jones (LJ) potential having a deep potential well and a short interaction radius. In the latter case, boundary i-atoms of Ti and Al (i.e. Ti and Al atoms bordering on the walls) experienced attraction to the walls (Fig. 1 (b)). The atoms forming the next atomic layer