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Study of mechanical properties of Ti-based intermetallides reinforced with carbon nanotubes

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The study is devoted to the study of mechanical properties under uniaxial tension and compression of polycrystalline structures based on intermetallic compounds of titanium aluminides ($TiAl_3$, Ti_3Al) and nickelide ($TiNi_3$) through molecular dynamic modeling. These alloys are of considerable interest as promising structural materials. The structural, elastic, and mechanical characteristics of these intermetallides reinforced with carbon nanotubes (CNTs) have been studied using the molecular dynamics method. The choice of CNTs as a reinforcing component is due to their unique properties, including high tensile strength, low density, significant modulus of elasticity and high aspect ratio. The results demonstrate that the introduction of carbon nanotubes significantly increases the mechanical strength of composites.

Keywords: polycrystal, modeling, mechanical properties, aluminides, nickelides.

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1. Introduction

The intermetallic compounds of the Ti-Al system are of considerable interest to modern high-tech industries due to their unique combination of physical and mechanical properties. These materials exhibit exceptionally low density ($3.7-4.0\,g/cm^3$), high specific strength that persists up to temperatures of $700-800\,^{\circ}C$, as well as outstanding resistance to oxidation and corrosion in aggressive environments [1]. This combination of characteristics makes them promising for use in critical components of aircraft engines, gas turbine installations and components of space technology, where the requirements for heat resistance and weight efficiency are particularly strict [1].

However, the practical use of titanium aluminides is hindered by a number of significant limitations. Studies in Refs. [2,3] show that these compounds have limited plasticity (elongation less than 2% at room temperature) and a tendency to brittle fracture, due to their complex crystalline structure (mainly type $L1_0$) and the covalent nature of interatomic bonds. In addition, the low diffusion mobility of atoms in an ordered lattice leads to significant technological difficulties in processing such materials using traditional methods [4].

Modern strategies for improving the properties of intermetallides based on Ti-Al compounds include several areas: 1) Doping with third elements (Cr, Nb, Mo, V), which makes it possible to modify the phase composition and deformation behavior of the material [5]. For example, the addition of $2-5$ at.% Nb significantly increases heat resistance and oxidation resistance. 2) Microstructural regulation through the creation of two-phase $(\gamma + \alpha_2)$ or ultrafine-grained structures [6]. 3) Composite approach with the introduction of dispersed reinforcing particles or reinforcing elements [7].

Titanium nickelides occupy a special position among modern functional materials due to the unique combination of mechanical characteristics and functional properties [8]. These intermetallic compounds exhibit outstanding characteristics, including superelasticity, high corrosion resistance, and biocompatibility, which determines their broad application prospects in various fields of engineering and medicine [9].

Of particular scientific interest is the study of the mechanical and strength characteristics of TiNi alloys depending on their phase composition and thermomechanical treatment [10].

A promising direction is computer modeling (using methods of molecular dynamics, finite elements, and DFT calculations), which studies the effect of reinforcing elements on the structure and properties of Ti-based intermetallides and their deformation behavior, which makes it possible to optimize their composition and reduce the volume of expensive experimental studies [11–13].

The purpose of this work is to study the effect of carbon nanotubes (CNTs) on the mechanical properties of titanium-based intermetallic compounds (Ti_3Al, $TiAl_3$ and $TiNi_3$) by the method of molecular dynamic modeling.

2. Modeling and results

In the framework of this study, models of polycrystals Ti_3Al and $TiAl_3$ with structures $D0_{22}$ and $L1_2$, as well as polycrystals $TiNi_3$ were created using open source software:

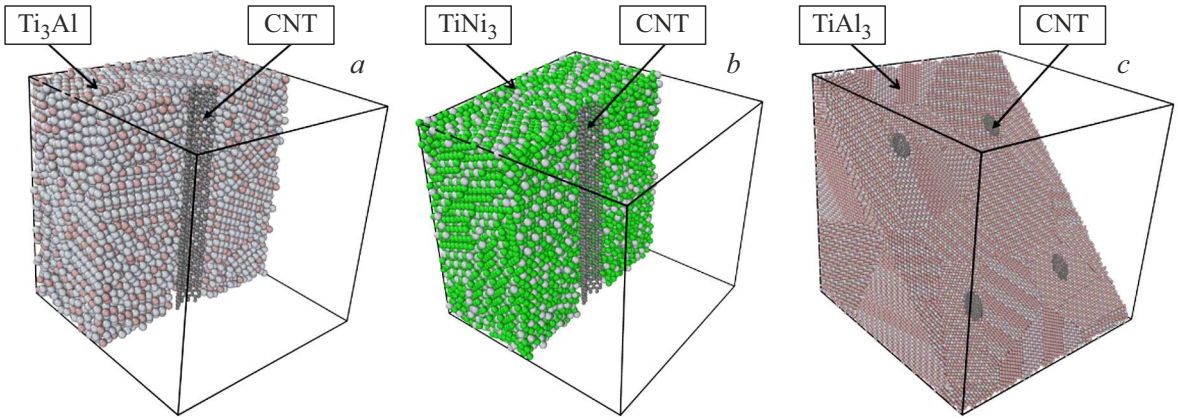

Figure 1. Models of intermetallic polycrystals (sections of computational cells): *a*) Ti_3Al-CNT; *b*) reinforcement scheme; *c*) $TiNi_3$-CNT; *d*) $TiAl_3$-CNT (with L1 structure$_2$).

Atomsk [14] utilities and large-scale atomic-molecular parallel the LAMMPS simulator [15]. Additionally, composite systems based on these intermetallides reinforced with CNTs of the „zigzag“ type were considered, while the volume fraction of CNTs did not exceed 5% of the total volume of the composite.

Polycrystalline structures were generated by the Voronoi method [16] with a random distribution of grain sizes and orientations. Modeling of composites containing CNTs assumed the creation of a metal matrix with cylindrical holes located along the entire height of the crystal. The diameter of the holes exceeded the diameter of the embedded nanotubes by 3 Å to ensure optimal interatomic interaction. Visualization of the simulation results was performed in the OVITO [17] software environment, including the analysis of structural defects and interatomic distances. Figure 1 shows models of polycrystals.

The accuracy of modeling uniaxial loading processes significantly depends on the correct choice of the potential of interatomic interaction in the composite material [18]. The corresponding MEAM potentials were used for intermetallic systems that do not contain carbon nanotubes (CNTs). However, to describe the interactions in CNT-reinforced composites, it is necessary to develop a hybrid potential that provides adequate modeling of interatomic interactions between carbon atoms, as well as between carbon and a metal matrix, as well as between the atoms of the matrix itself. The adaptive intermolecular reactive empirical bond order (AIREBO) potential was used to describe the carbon–carbon interaction. The Lennard–Jones potential was used to describe the interaction of carbon with the atoms of the metal matrix (for Ti, the parameters are derived from [19], for Al from [20], and for Ni — [21]):

$$V(r) = 4\varepsilon[(\sigma/r)^{12} - (\sigma/r)^{6}].$$

The EAM potential selected in the NIST database [22] was used to describe the interaction between the atoms of the matrix. The total energy of the system has the form:

$$E_{\text{total}} = E_{M-\text{M}} + E_{\text{C}-\text{C}} + E_(M - \text{C}),$$

where $E_{M-\text{M}}$ and $E_{\text{C}-\text{C}}$ describe the potential energies of the metal matrix and carbon nanomaterials, respectively, and $E_{M-\text{C}}$ is the interaction between metal and carbon atoms. The equation for the total energy of the system is given to demonstrate the completeness of the approach used, although further analysis focuses on the mechanical characteristics resulting from this energy description.

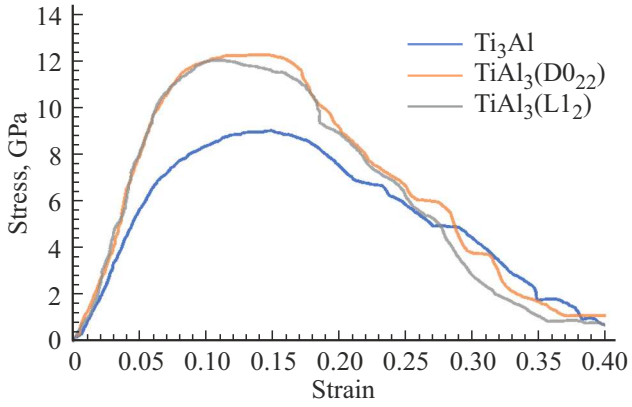

Figure 2. Stress/strain curves during uniaxial stretching of polycrystals at a temperature of 300 K.

Figure 2 shows the result of uniaxial loading for polycrystals Ti_3Al and $TiAl_3$ in two phases: $D0_{22}$ and $L1_2$. Mechanical properties such as ultimate strength and yield strength have a higher value for $TiAl_3$ intermetallic compound, and these values are slightly higher for the $D0_{22}$ phase. As for the Young's modulus, the values differ slightly: 109.81 GPa — Ti_3Al; 115.91 GPa — $TiAl_3$.

Further research was aimed at studying the reinforcing effect of CNTs. The following results were obtained when introducing 3% volume fraction of CNTs in the composite:

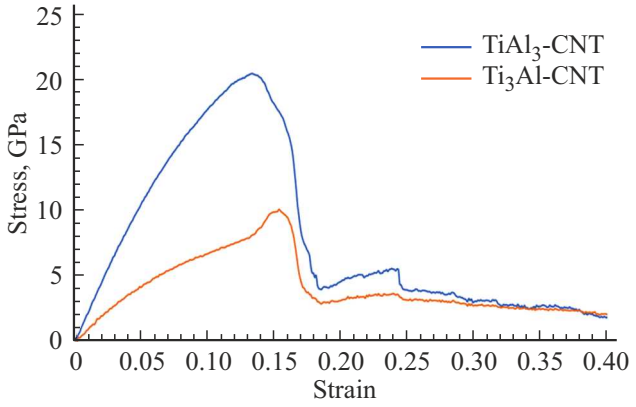

Figure 3. Stress/strain curves under uniaxial stretching of composites at a temperature of 300 K.

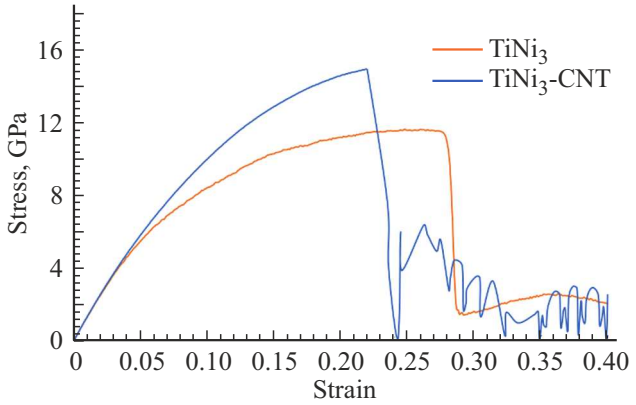

Figure 4. Stress/strain curves under uniaxial tension of $TiNi_3$ intermetallic compound and composite $TiNi_3$-CNT.

the Young's modulus for the composite Ti_3Al-CNT was 159.8 GPa; the Young's modulus for $TiAl_3$ was 215.81 GPa. Figure 3 shows the result of uniaxial stretching of composites. The ultimate strength for the Ti_3Al-CNT composite increased by an insignificant value by 0.5 % compared to „pure" polycrystal. For the composite $TiAl_3$-CNT, the increase in tensile strength is already significant — 43 %.

Atomic modeling of uniaxial stretching of titanium nickelide and CNT-reinforced composite was carried out at a temperature of 300 K and constant pressure. The result is shown in Figure 4.

There is an increase in tensile strength by 23 %. However, the elastic deformation phase for a CNT-reinforced composite is shorter compared to a pure polycrystal.

3. Conclusion

It has been established by the method of molecular dynamic modeling that the intermetallic compound $TiAl_3$ (phase $D0_{22}$) exhibits higher values of ultimate strength and yield strength compared with Ti_3Al, which is consistent with its more rigid crystal structure. At the same time, the Young's modulus of both compounds turned out to be close: 109.81 GPa for Ti_3Al and 115.91 GPa for $TiAl_3$. The introduction of 3–5 % of the volume fraction of CNTs into the matrix of intermetallides leads to a significant improvement in their mechanical characteristics. So, an increase of Young's modulus by 86 % (up to 215.81 GPa) and increase of tensile strength by 43 % is observed for $TiAl_3$-CNT. The Young's modulus increases by 45 % (to 159.8 GPa) for Ti_3Al-CNT, however, the tensile strength increases slightly (+0.5 %), which may be due to the peculiarities of the interatomic interaction at the „metal matrix — CNT" boundary.

In the case of $TiNi_3$, CNT reinforcement increases the ultimate strength by 23 %, but reduces the elastic deformation phase, which indicates a change in the plasticity mechanism — this effect requires further study for use in biomedical shape memory alloys.

The simulation results confirm that carbon nanotubes effectively block the movement of dislocations, especially in the $TiAl_3$ intermetallic compound, where their effect is most pronounced. This is attributable to the high rigidity of CNTs and strong bonding at the interface.

The results obtained can be used for new generations of intermetallic composite materials with specified mechanical properties.

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Conflict of interest

The authors declare that they have no conflict of interest.

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