

Mathematical Model of Intermetallic Phases Formation inside a Nickel Surface Layer under Implantation of Aluminum Ions

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Abstract – A mathematical model, which describes interaction of high intensity aluminum ion beams with nickel targets, is proposed. Results of modeling and their comparison with experimental data are discussed.

1. Introduction

Nowadays, synthesis of intermetallic nanoparticles inside metallic targets under ion implantation for producing materials with high physical mechanical and tribological behavior has a great practical importance. Interest to this problem is due to unique characteristics of intermetallic compounds. At high temperature, they, besides structural stability and durability, have good anticorrosion and antifriction characteristics, which are better than those of construction alloys [1].

Creation of intermetallic structures in a nanocrystalline state in surface layers can be performed with success by influence of high intensity ion beams on the surface atoms. At that, the dominant factors affecting the phase formation and the depth distribution of implanted impurities inside targets are the ion current average density (>0.1 mA/cm²) and ion flux (dose) ($>10^{17}$... 10^{18} ion/cm²) [2]. It has to be noted that the ion synthesis is a complicated physical chemical process. Physical-chemistry characteristics of implanted layers depend on implantation condition and can change in a wide range.

Studying the physical chemical correlations, the processes of creating ion alloyed metallic layers with nano intermetallic components in the process of a high intensity metallic ion implantation is very important present-day task. A theoretical aspect of this investigation is also important because it would be possible to develop a model of creating the structural phase state of the target surface layer while irradiated by metal ions, especially in the high intensity regime.

The object of our work is to investigate the microstructure and phase composition of nickel surface layers at different conditions of aluminum ions implantation and to develop the theoretical model of the processes at high intensity ion implantation. We have studied the nickel samples implanted by aluminum ions in order to produce modified layers of high heat resistance and durability.

2. Materials and investigation methods

Ion implantation targets were made from a polycrystalline nickel. A high intensity aluminum ion implantation in nickel was accomplished by a vacuum arc ion plasma source "Raduga-5" [2, 3]. An accelerating voltage was 40 kV. The distance between the source and samples was (0.24...1.04 m) and an implantation temperature was in the range (450...1600 K) [3, 4]. The different source-sample distance changes the ion dose in the range ($4 \cdot 10^{17}$... $8.3 \cdot 10^{19}$ ion/cm²) [3, 4]. We used the Rutherford back scattering (RBS) and transmission electron microscopy (TEM) to investigate the element composition and structural phase state of the implanted nickel samples.

3. Experimental results

In accordance with the RBS method, the ion alloyed layer thickness increases with the irradiation dose. Under implantation dose at $4 \cdot 10^{17}$ ion/cm² the implanted surface layer thickness was 150 nm. The thickness increases with dose up to 350 nm (irradiation dose was $2 \cdot 10^{18}$ ion/cm²) and up to 1000 nm (irradiation dose was $1 \cdot 10^{19}$ ion/cm²). An implanted aluminum maximum concentration in metallic matrixes was 60...70 at. %.

With a micro diffraction analysis of the surface ion alloyed layers we have found that fine-dispersed phases of a Ni-Al system are generated as a result of the ion irradiation: γ -phase (solid solution of Al in Ni), γ' -phase (inter metallide Ni₃Al), and β -phase (inter metallide NiAl) [3–5]. The solid solution (γ -phase) has a face-centered cubic lattice, γ' -phase is a well-ordered phase with a super structure L1, based on FCC lattice, and β -phase is a well-ordered phase with a super structure B2 and body-centered lattice [5]. In all regimes, we have observed creation of nano intermetallic phases, the grain average size being 24...65 nm.

The composition, ratio and phase localization through the depth of alloyed layers depend on the implantation conditions. Comparison of aluminum concentration profiles in nickel matrixes and the phase diagram of the Ni–Al [3–5] system show the localization of phases created by ion implantation.

We have established a general pattern of localization structure of intermetallic phases and solid solutions through the depth of implanted layers. With growing depth, we have observed three regions smoothly transforming in each other: there are a three-phase (Ni₃Al, NiAl, and solid solution), a two-phase (NiAl and solid solution), and a single-phase (solid solution) regions.

4. Mathematical model

Let us assume that an h -thickness nickel plate irradiated by a uniform ion flux is in an ideal heat contact with a copper substrate. A total system of equations, describing the ion-plasma treatment (aluminum ions) of the nickel plate, includes a heat conduction equations with a chemical heat source for every layer (nickel and copper) and kinetic equations for the reaction components. In general, the problem is both conjugate (the border between materials) and combined (an interaction between concentration and temperature fields is under consideration). Large mathematic recourses are needed for its numerical solution even for a single dimension problem due to the difference of thermal and diffusion scales. However, this circumstance can be used to simplify the problem.

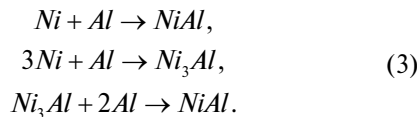
Indeed, for solids:

$$x_d \ll x_T, \quad (1)$$

$x_d = \sqrt{Dt}$ is a diffusion zone width in a characteristic time t ; $x_T = \sqrt{\kappa_T t}$, is the width of a warming-up zone in nickel, $D = D(T)$ is the ion diffusion coefficient for nickel; κ_T the nickel heat conductivity coefficient. The following condition usually holds:

$$x_T \geq h. \quad (2)$$

In accordance with general conceptions, we have:



Taking into account diffusion of aluminum atoms into nickel, we have the following system of kinetic equations:

$$\frac{\partial y_3}{\partial t} = \frac{\partial}{\partial x} D(T) \frac{\partial y_3}{\partial x} + b^{-1} \rho V_3 m_3^{-1} F(t, x) + \sigma_3, \quad (4)$$

$$\frac{dy_2}{dt} = \sigma_2, \quad \frac{dy_1}{dt} = \sigma_1, \quad \frac{dy_4}{dt} = \sigma_4,$$

y_1 is concentration of NiAl, y_2 —Ni₂Al, y_3 —Al. A concentration dimension is mole/m³. In an open system: $y_1 + y_2 + y_3 + y_4 \neq \text{const}$.

An external source is taken from the dimension consideration. A function includes experimental parameters.

$$F(x, t) = f(t) \exp\left[-\left(\frac{x-a}{b}\right)^2\right],$$

V_k is a maximum speed of k -ions in surface layers. Parameters b and a for different ions can differ. The

function F shows the decrease of ion speed in the surface layer due the processes, which are not manifested in the model. This function dimension is mole/(m³c).

Internal sources and wells can be expressed as follows:

$$\sigma_k = \sum_{i=1}^3 v_{ki} \varphi_i, \quad k = 1, 2, 3, 4,$$

v_{ki} is a stoichiometrical coefficient of a k – component in i -reaction, φ_i is the rate of i -chemical reaction [mole/(m³c)].

In accordance with (3):

$$\sigma_1 = \varphi_1 + \varphi_3; \quad \sigma_2 = \varphi_2 - \varphi_3;$$

$$\sigma_3 = -[\varphi_1 + \varphi_2 + 2\varphi_3]; \quad \sigma_4 = -[\varphi_1 + 3\varphi_2].$$

In accordance with an acting mass law and the Arrhenius law, we can represent the chemical reaction rate function as follows:

$$\varphi_1 = k_1 y_3 y_4, \quad k_1 = k_{10} \exp\left(-\frac{E_1}{RT}\right),$$

$$\varphi_2 = k_2 y_3 y_4^3, \quad k_2 = k_{20} \exp\left(-\frac{E_2}{RT}\right),$$

$$\varphi_3 = k_3 y_2 y_3^2, \quad k_3 = k_{30} \exp\left(-\frac{E_3}{RT}\right),$$

k_{10} , k_{20} , k_{30} are preexponential factors, E_1 , E_2 , E_3 are the reaction activation energies. We assume that all parameters are known whether from experiments or from independent calculations.

Taking into consideration (1, 2, and 4), we have:

$$c_b \rho_b \frac{\partial T_b}{\partial t} = \frac{\partial}{\partial x} \left(\lambda_b \frac{\partial T_b}{\partial x} \right), \quad (5)$$

$$\begin{aligned} -\lambda_b \frac{\partial T_b}{\partial x} &= q_0 \frac{\sqrt{\pi}}{2} f(t) \text{erf}(bh + a) - \\ x=0: & -\varepsilon \sigma (T^4 - T_e^4) + \int_0^h \sum_{i=1}^3 Q_i \varphi_i dx - hc \rho \frac{dT}{dt}, \end{aligned} \quad (6)$$

$$x = H: \quad -\lambda_b \frac{\partial T_b}{\partial x} = A(T_e - T_b) + B, \quad (7)$$

$$Q_e = b^{-1} \rho h_3 V_3 m_3^{-1} F(t, x) = b^{-1} q_0 F(t, x),$$

$q_0 = \rho h_3 V_3 m_3^{-1}$ is a maximum heat flux density due to the implanted ions.

$$Q_1 = -(h_4 + h_3 - h_1); \quad Q_2 = -(3h_4 + h_3 - h_2);$$

$$Q_3 = -(2h_3 - h_1)$$

are the reaction heat effects.

h_k is partial enthalpy, σ is the Stefan-Boltzmann constant, ε is a blackness index, y_{30} is an aluminum quantity in plasma, α_m is the mass exchange coefficient, λ_b is a copper thermal conductivity [Joule/(cm·s·K)].

We assume a general boundary condition on the external side of a copper substrate in order to control the sample cooling. $T = T_b(0, t)$ is a nickel target temperature.

At zero moment:

$$t = 0: T = T_0; y_4 = 1; y_1 = y_2 = y_3 = 0. \quad (8)$$

We assume that the Arrhenius law holds:

$$D(T) = D_0 \exp\left(-\frac{E}{RT}\right), \quad (9)$$

D_0 is a preexponential factor, E is a diffusion activation energy.

5. Conclusion

We have investigated the element composition and structural phase state of nickel surface layers alloyed by aluminum ions. At that, the layers with thickness up to 1 μm are produced. Modified surface nickel layers contain the fine-dispersed intermetallic Ni_3Al and NiAl phases and a solid solution with alternating depth composition. The Ni-Al system state diagrams correspond to creation of intermetallic phases. We have found localizations of phases created in the implantation process through the depth of

ion alloyed metal layers. We introduce a mathematical model of phase formation processes by ion implantation. The mathematical model has proved to be correct.

References

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