ON THE MICROSTRUCTURE AND MECHANICAL PROPERTIES OF NANOCOMPOSITES

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Keywords: *Aluminium alloys, nickel alloys, crystal structure defects, SiC, nanodiamonds*

Abstract: *The present study reports the effects of the microstructure parameters and thus the mechanical properties of nanostructured aluminium, and nanostructured nickel. We study the possibilities for strengthening of aluminium, nickel, aluminium alloys and nickel alloys on the basis of analysis of their microstructure properties. We review the main crystal structure defects responsible for strengthening of aluminium alloys. A critical discussion is presented. Possible extensions of this work in the future are considered.*

ОТНОСНО МИКРОСТРУКТУРАТА И МЕХАНИЧНИТЕ СВОЙСТВА НА НАНОКОМПОЗИТИТЕ

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Ключови думи: *Алуминиеви сплави, никелови сплави, дефекти на кристалната структура, SiC, нанодиаманти*

Резюме: *Разгледани са ефектите на микроструктурните параметри върху механичните свойства на наноструктуриран алуминий и наноструктуриран никел. Ние проучваме възможностите за укрепване на алуминий, никел, алуминиеви сплави и никелови сплави въз основа на анализ на свойствата на тяхната микроструктура. Прави се преглед на основните дефекти в кристалната структура, отговорни за укрепването на алуминиеви и никелови сплави. Дискутират се резултатите, правят се изводи и се разглеждат бъдещи изследвания.*

Introduction

The report is motivated by the very modern nowadays nanoscience, nanotechnology and nanocomposites. Nanostructured objects, and especially nanostructured metals, alloys and composites, are now intensively investigated by many foreign and bulgarian scientists [1-16]. Here the subject of the study are aluminum and nickel, and alloys on their basis, and also composites based on Al, and Ni.

In nanoscience computer simulations and modeling (which is an important component of modern science) are particularly useful. They complement, develop and connect theory and experiment and technology. Of course, pure theoretical science can not always completely solve technical problems, as its methods are systematically related to the simplification of processes and phenomena. But today science can predict many of the properties of substances from their composition. Here we also examine the possibilities for the application of computer modeling of the structures already mentioned.

The information contained in this study has been compiled from the literature and it may be considered as a first part of an introduction to the subject mentioned above.

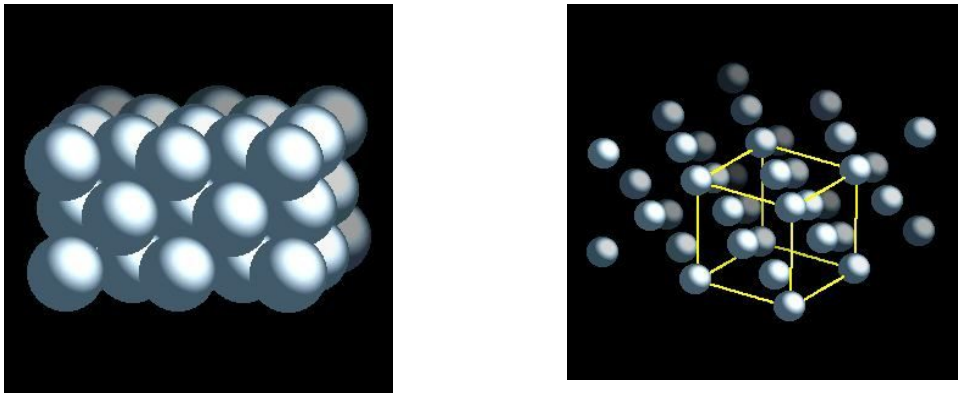
Structure parameters and properties of Al and Ni

In this work we present the data on the structure of aluminum (Al) and nickel (Ni), and their alloys very briefly, since these data are widely represented in the literature.

Aluminum is a metal of the third A group of the periodic system of elements and its alloys are characterized by high electrical and thermal conductivity. Al has a melting point of 658.7ºC. The most common elements in aluminum alloys are copper, zinc, magnesium, manganese and silicon. Al has a metal structure with atoms arranged in a face centered cubic crystal lattice (fcc), structural type A1, space group Fm3m, coordination numbers 12, lattice parameter of 4.0496 Å, interatomic distances 2.863 Å, 2.698 g/cm^3 density, atomic radius of 1.43 Å, the volume of an atom 16.60 Å^3. High strength deformable aluminium alloys have high strength (600-700 MPa), but they are not plastic, and at temperatures above 150°C, have falling values for their strength and corrosion resistance Interest in these fcc metals is so great, as most of the experimental data was obtained for these metals. The defects of the crystal structure and mechanical properties are considered together, although these defects determine not only mechanical properties of metals and alloys, but also a number of important physical characteristics. For example, the increase in the density of dislocations increases internal friction, changes optical properties, increases electrical resistance of metals. Dislocations increase the average speed of diffusion in crystals, accelerate aging and other processes related to diffusion. Mechanical and tribological properties are part of the physical properties of substances. The presence of certain mechanical / tribological properties is one of the main requirements for metals and alloys, which is explained by their ability to serve as a structural material in various fields. For example, aluminum alloys, which are widely used as materials in aeronautical engineering must be able to withstand the following conditions: high speeds, rapidly changing external power influences cyclical peak loads, large temperature differences.

Dislocations in crystals are one of the most important structural defects that are relevant to their strengthening. For example, in real fcc crystals the full resistant dislocations are with: Burgers vector 1/2 <110>; slip direction of <110>; most commonly observed slip planes of {111} [18,19]. Often, but not always, the slip planes are the most densely packed planes. One of the most important properties and peculiarities of the structure are the defects of the crystal lattice - vacations, dislocations, stacking faults, impurity atoms, etc. When we talk about the influence of structure on the properties, we above all mean dependence on the structure defects. Almost all properties are structurally sensitive. And all the properties are dependent on the phase composition, i.e. composition and phases. Impurity components in their pure form are isovalent and their atomic volumes are different from those of the matrix. Impurity atoms in the crystal lattice are distributed irregularly and are concentrated on the structural defects.

Dislocations, besides being possible type of defects in the crystal lattice, are extremely important for a number of practical problems. The density of dislocations is defined as the amount of dislocations that intersect any section of the crystal area of 1 cm^2. Or another way: the density of dislocations can be defined as the sum of the lengths of dislocation lines in 1 cm^3. Mechanical strength and plasticity of solids mainly depends on dislocations. The influence of dislocations on the strength of the material is most easily explained by analyzing the stress-strain diagram (Diagram strength / stretching) [19]. In the application of a load we have two processes associated with dislocations: generation of new dislocations and relocation / movement of existing and newly created dislocations. Macroscopic speed of deformation of a crystal is determined by the density of moving dislocations and their average speed at a given load [18, 19].



Фиг. 1. Structure of Al

Nickel is a chemical element with the chemical symbol Ni and atomic number 28. It is a silvery-white lustrous metal with a slight golden tinge. Nickel belongs to the transition metals and is hard and ductile. Pure nickel shows a significant chemical activity that can be observed when nickel is powdered to maximize the exposed surface area on which reactions can occur, but larger pieces of the metal are slow to react with air at ambient conditions due to the formation of a protective oxide surface. Even then, nickel is reactive enough with oxygen. Because of nickel's slow rate of oxidation at room temperature, it is considered corrosion-resistant. Historically this has led to its use for plating metals such as iron and brass, to its use for chemical apparatus, and its use in certain alloys that retain a high silvery polish, such as German silver. The metal is chiefly valuable in the modern world for the alloys it forms; about 60% of world production is used in nickel-steels (particularly stainless steel). Nickel has a melting point 1455°C. Nickel is a transition metal of a group 10 of the periodic system of elements. Ni has a metal structure with a fcc crystal lattice (face centered cubic crystal lattice, see fig. 2 [17]), structural type A1, space group Fm3m, coordination numbers 12, lattice parameter of 3.524 Å, interatomic distances 2.492 Å, 8.96 g/cm^3 density, atomic radius of 1.24 Å.

Fig. 2. Highly purified nickel spheres [17]

Nickel based composites

A composite is a material comprised of two or more physically distinct materials with at least one material providing reinforcing properties on strength and modulus. Composite materials (KM) or multicomponent materials are composites consisting of a base / matrix reinforced with the reinforcement / fillers (which may be fiber strands, particles, etc.). By selecting the composition and the properties of the matrix and reinforcement, and processing route, one receives materials with necessary combination of exploitation and technological properties.

We can distinguish two types of nickel based nanostructured KMs: bulk or surface nanostructured (nanostructured nickel based coatings). In both types of nickel KMs, one can use various substances as reinforcements (B, BN, nanodiamond, SiC, graphite, diamond and SiC, TiC, TiN, TiCN, Al_2O_3, ZrO_2, TiO_2, etc.). Nanostructured Ni based coatings are widely spread and used, and very popular in surface modification, giving rise to production of coatings with new, improved, desirable, high quality and tailoring surface properties for various applications.

Now let’s consider the possibilities to increase the strength characteristics of Ni composite by adding to nickel nanodiamond or SiC (silicon carbide). These reinforcements are used for production of corrosion and wear resistance surfaces.

For example, we will compare their melting temperatures, which are as follows: Ni (1455 °C) (for bulk Ni), Ni (approximately 880 °C) (for electroles Ni), SiC (2540 °C) nanodiamond (600 °C). It is clear that to operate at higher temperatures is preferable to choose SiC.

In terms of the combination of micro hardness and brittleness, must again look into SiC. Nanodiamonds are hard but brittle under load, unlike SiC. SiC microhardness is 33 GPa.

As to the densities, they are approximately equal and therefore theoretically equivalent: SiC (3,2 g/cm^2) and nanodiamond (about 3 g/cm^2).

Lattice parameters of Ni, SiC and nanodiamond are respectively equal to: 0.352 nm; 0.44 nm and 2.5 nm. Basically nanodiamond sizes are from 4 nm to 6 nm. But nanodiamonds are conglomerates of atoms. It is not clear how to do their incorporation into the Ni matrix, so as to preserve their integrity. Embedding depends on the applied technology of obtaining composite. And in

all cases, increasing the dimensionality of the solid phase is making more difficult the movement of dislocations in the matrix. And this in turn leads to the increase of the strength.

It should be noted that the smaller are individual crystals of Ni matrix, the greater is the hardness of the composite.

In the literature there are sufficient data for such a strengthening of Ni with nanodiamonds (ND) and SiC.

The [6] study reports the effects of electroplating parameters on the microstructure and thus, the mechanical and tribological properties of nanostructured nickel. Results show that electroplating produced thick, dense and uniform nickel deposits with grain size down to 10's of nm and a length/width ratio around 1.8. The grain size and distribution were found to significantly affect hardness and elastic properties with the smallest grain size possessing a hardness that was at least three times higher than that of bulk nickel. Nanostructured nickel showed lower coefficients of friction and wear rates compared to that of bulk nickel and the nanostructured nickel with the smallest grain size exhibited the lowest coefficient of friction and wear rate. These differences were attributed to different wear mechanisms. Bulk nickel showed extensive cracking and evidence of material removal under a wear fatigue mechanism. On the contrary nanostructured nickel exhibited a fine abrasive wear mechanism. This study presents results that suggest a consistent relationship between processing parameters, grain size and distribution, hardness, and wear behavior in electroplated nickel. Understanding of this relationship can be applied to tailor properties and improve behavior of MEMS components. In this study nanostructured nickel samples were electrodeposited under various conditions and characterized by microstructural, mechanical and tribological properties in an effort to develop a better understanding of processing-structure-property relationship.

Fundamental investigations on the origins of friction at the nanoscale were carried out in [7] using both theoretical and experimental approaches. A model was developed that analytically solves for friction by the motion of dislocations at atomically flat crystalline interfaces.

The paper [8] reviews the properties of the electroless nickel deposits and describes successful applications.

Computer modelling can lend valuable support to experimental and theoretical research on fracture mechanisms. The paper [9] describes examples of the modelling of brittle .tracture in bcc metals, where the preference for the {100} cleavage plane can be explained, and various applications of computer modelling to the mechanisms of toughening brittle materials by ductile inclusions. Computer modelling is beginning to make important contributions to the understanding of fracture processes in metals and composite materials, in the sense that it has become possible to predict the behaviour of materials in microregions which are not, or not completely, accessible to experiment.

The study [10] describes the development of multilayer metal-dielectric graded index solar selective coatings in which the metallic volume fraction increases with depth, from top (air–film interface) to bottom (film–substrate interface). The work is based on computer simulation followed by validation through fabrication of the coatings and optical measurements.

Al matrix composites (AMCs)

Here we concentrate on metallic KM based on Al. As reinforcements can be used various substances (graphite particles [13,14], B, nanodiamond, SiC, diamond and SiC [15], TiC, Al_2O_3, ZrO_2, molybdenum coated nanotubes, etc..), But here we consider only three the possibilities: nanodiamond [12], SiC (silicon carbide) [11] and diamond with SiC [15]. Better performance has AMC with added SiC, than that of nanodiamond. The addition of SiC is preferred over ultradispersed detonation nanodiamond when it comes to increasing the strength characteristics of Al composite. For example, we will compare their melting temperatures, which are: Al (660^{o}C), SiC (2540°C), nanodiamond (600°C). It is clear that to operate at higher temperatures is preferable to use more churlish reinforcement. In this case this is SiC. In terms of the combination of micro hardness and brittleness, must again look into SiC. Nanodiamonds are hard but brittle under load, unlike SiC. SiC microhardness is 33 GPa.

As to the densities, they are approximately equal and therefore theoretically seems equivalent: SiC (3,2 g/cm^2) and nanodiamond (about 3 g/cm^2).

Lattice parameters of Al, SiC and nanodiamond are respectively equal to: 0,4 nm; 0,44 nm and 2,5 nm. Basically nanodiamond sizes are from 4 to 6 nm. But nanodiamonds are conglomerates of atoms. It is not clear how to do their incorporation into the matrix Al, so as to preserve their integrity. Embedding depends on the applied technology of obtaining composite. And in all cases, increasing the dimensionality of the solid phase makes more difficult movement of dislocations in the matrix. And this in turn leads to the increasing of strength.

It should be noted that the more small individual crystals of Al matrix, the greater is the hardness of the composite.

In the literature there are sufficient data for such a strengthening of Al with nanodiamonds (ND), diamonds and SiC.

For example (see Figure 2.) [12] with the increase of the concentration of the nanodiamond in Al composite hardness of the metal composite is also growing. For example, Fig. 3 [11] shows the variation of cumulative wear volume with normal applied loads; volume loss is increasing with increasing normal loads. Wear volume loss is maximum for pure aluminium and then decreases as the % SiC increases up to 20%. Again this trend changes for 25% SiC content because of non-uniform mixing.

The diamond/SiC/Al composites with high volume fractions and a large ratio of diamond to SiC particle size (7.8:1) were fabricated and investigated in [15]. The results show that the fine SiC particles occupy efficiently the interstitial positions around coarse diamond particles; the main fracture mechanism of the composite is matrix ductile fracture, and diamond brittle fracture was observed which confirms a high interfacial bonding strength; the diamond/SiC/Al composites with 80% and 66.7% volume fraction of diamond in the reinforcement have the higher volume fraction in the reinforcement and lower coefficient of thermal expansion compared to the diamond/Al composite. Turner and Kerner models are not in good agreement with the experimental data for the composites based on reinforcement with two phases different in shape and component. When the effect of the coating layer considered, differential effective medium (DEM) model is confirmed a reliable model in designing a composite with a given thermal conductivity based on reinforcement with two phases different in size.

Conclusion and future work

In this paper we presented an introduction to the connection of microstructure and mechanical properties of nanostructured aluminium and nickel. We see the important role of different reinforcements in the tailoring of mechanical properties of composites. In the future could be considered new and still unfulfilled combinations of various reinforcing additives to the Al and Ni matrix. Work can proceed with reinforcement of Al and Ni with three phases at the same time as reinforcements. Possible extensions of this work may be investigation of:

- consideration of all possible substances as reinforcements in Al- and Ni matrix composites, comparing their parameters and selection of the most suitable for specific applications (aerospace and other applications);
- calculation of the structural characteristics of the data and planning an experiment to verify the validity of the calculations.

Theoretical calculations can significantly contribute to determine the optimal parameters for various combinations of reinforcement phases or possible and optimal composite coatings, to obtain the desired properties and design of the composite. As in [16], where are applied ANOVA and ANN modeling techniques to optimize the parameters of Al / SiC composites. The future studies, which focus on how nanostructured materials perform and how the microstructures affect their properties, will make the process of customizing these materials easier.

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