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Multiscale modelling of aluminium-based metal–matrix composites with oxide nanoinclusions

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ABSTRACT

In this work, we study the dependence of Young’s modulus and the strength of aluminium-based metal–matrix composites from the volume fraction of inclusions and the size of oxide inclusions dispersed in the matrix. We consider the metal–matrix composites containing extremely low volume fraction of oxide inclusions (<0.15%) with the inclusion size from 30 nm to 600 nm. We analyse the non-monotonic experimental dependences of the mechanical properties from the volume fractions of inclusions and the inclusions size, which reflect the scale effects. We study the effective properties and yield strength of the filled aluminium-based metal–matrix composites with spherical inclusions and take into account the possibility of agglomerates formation from the inclusions. To describe the anomalous behaviour of materials with saturated internal structural heterogeneity, the gradient theories are involved. As a result, in this work, on the basis of the gradient elasticity, the self-consistent method of three spherical bodies and the method of radial multipliers, we provide the modelling of experimentally observed effects of scale amplification of the mechanical characteristics of the metal–matrix composites depending on the volume fraction of the particles. The theoretical modelling uses the idea of the interphase layer and demonstrates correspondence to the experimentally observed effects of scale amplification of mechanical characteristics for the aluminium-based metal–matrix composites reinforced by the extremely low volume fraction of oxide inclusions. Based on a comparison with experimental data, the additional parameters of the non-classical models are determined, which helps to explain the impact of scale effects (the size of the inclusions) on the properties of composites.

1. Introduction

Aluminium metal–matrix composites reinforced with ceramic particles are widely used in aviation and aerospace because of low density, high strength and workability [1–3]. Using nano-sized particles as fillers leads to a significant increase in the functional properties of powder materials, since they have a considerable influence on the sintering process activation, matrix grain shredding, dispersion strengthening, decrease in porosity and so on. Many research studies in the field of aluminium composites reinforced by ceramics nanoparticles were carried out in the event of significant concentrations exceeding 1% of volume [4–10]. There are few works in which the assessment of the impact of nanoparticles on the material properties was carried out for the concentrations of 0.25% and higher [11,12]. However, it remains a little-studied problem – the influence of nanoparticles on the properties of alloys in case of very small concentrations. The literature has often noted that with an increasing concentration of nanoparticles of up to 10%, a particular property of the material changes dramatically, having one extremum in the property/concentration diagram. In the recent studies of composites [8–10] manufactured by powder metallurgy, based on the matrix of the aluminium alloy and hardened different nanoinclusions, the substantial increase in strength of composites was found in concentrations of 1–5%. In Ref.

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[8], the composite based on aluminium matrix, with filling from 1 to 7 vol.% by nanoparticles of Al_2O_3 of size 50 nm, which were located along the matrix grain boundaries and formed clusters of size up to ~100–400 nm was investigated. When the content of oxide was 0%–4%, aluminium grain size decreased. However, for concentrations above 4%, the grain size stabilized at the level of 1.2 μm. The reason, apparently, is an effect of saturation of nanoparticles on the grain boundaries. In Ref. [9], a significant reduction in the porosity and an increase of strength were observed for composites with nanoinclusions of Si_3N_4 with a diameter of 15 nm and a concentration of 1%. The mechanical properties of aluminium, hardened with aluminium oxide nanoparticles (60–200 nm) and silicon carbide (60–200 nm) with volume content within 1–5%, were studied in Ref. [6]. It is shown that the volume content and the size of nanoparticles have a significant effect on the porosity and hardness of the composite. Composites based on aluminium alloy A356.1, hardened with MgO nanoparticles containing 1.5; 2.5; 5 vol.%, were considered in Ref. [7] and the 'jump' of the composite strength under compression has been discovered for concentrations of 1.5 vol.% MgO. In Ref. [10], a metal–matrix composite based on alloy AA7075, hardened with silicon carbide nanoparticles in a concentration of 1 vol.% and 5 vol.% SiC, was studied. The diameter of the nanoparticles was 50 nm. The maximum values of tensile strength (630 MPa) and the yield strength (600 MPa) are observed in the case of low concentrations (1 vol.% SiC). The difference of the present work is that we study and simulate the aluminium matrix composites modified by the zirconia nanoinclusions in which reinforcement effect has been found experimentally for the small volume of fractions of nanoinclusions of up to 0.01–0.2%. And it is typically observed that effective property tends to increase with increasing concentration of nanoparticles from 1% to 10% of volume content, while having a pronounced extremum in the property/concentration diagram. In this paper, we discuss the results of experimental studies of the influence pointed to the existence of second extremum, which appears at an extremely low concentration of inclusions (in the order of hundredths and thousandths of a percent). Such reinforced scale effects require explanation. The essential problem is the construction of theoretical model of metal composite deformation with ultra-low content of the nanoinclusions, because the direct use of classical methods of composite mechanics does not allow to explain the scale effects.

There are a lot of works in the area of modelling of metal–matrix composite properties and stress–strain state under different types of loading. The investigation of size effects on the mechanical properties of particle-reinforced metal–matrix composites was studied in the recent works with analytical and numerical models [13–15]. Clustering effects were studied in [15,16]. Influence of interphase and interface strength between metal–matrix and ceramics inclusions were studied in many works [17–20]. Usually, the numerical approach based on the finite element models with cohesive zone elements and coated inclusion models is used in these works.

In the present paper, we develop a model that explains the reinforced effects of using a gradient theory of elasticity. The dependence of the effective elastic modulus and metal composite strengthening are simulated not only from the volume content of the inclusions but also from the effective size of the inclusions, the interphase zones around inclusions, mechanical properties of the interphase zone and its size. It is proposed to explain the anomalous properties of the metal composite reinforced with ultra-low volume fraction of the nanoinclusions of ZrO_2, by the interphase layer and special properties of the interface between the matrix and the inclusion. For the descriptions of the scale effects of metal composite, we propose to take into account the possibility of the most dense packing implementation of the disperse nanoinclusions surrounded by interphase layers. These effects are displayed with a high degree of the dispersion. It is assumed that these effects of 'saturation' occur, when the surrounded nanoinclusions in the interphase zones of altered morphology begin to overlap with each other.

In the first part of the work, the algorithm of modelling of effective nanocomposite properties based on the gradient elasticity theory and the method of self-consistent phases of Eshelby–Christensen is presented. The length of the interphase layer is determined by the gradient parameter of the model. Then, a model of the formation and growth of clusters depending on the inclusion concentration is introduced; and the evaluation of the radius around inclusions taking into account the saturation effects is given. Then, the model parameters are specified, using the analysis of the experimental data, and a modelling of effective elastic modulus of metal composite is brought. It also presents a variant of reinforced effect modelling based on the considering of the four-phase model of the inclusion with an additional interphase layer in the method of self-consistent phases for the classical theory of elasticity. In the last part of the paper, a numerical simulation of the scale-reinforced effect for the considered composite by the finite element method is given. It is shown that taking into account the characteristics of the interphase layer and the parameters of the clustering process allows to describe the effects of non-monotonic behaviour of the elastic modulus and the strengthening of the composite with the change in the volume content of the inclusions adequately with numerical simulation.

The aim of the article is to simulate the effects of the significant changes in the properties of aluminium-based metal–matrix composites under the ultra-low concentrations of nanoscaled inclusions. A brief description of the technique of carrying out the experimental tests and the experimental data are presented below.

2. Experimental tests for aluminium-based metal–matrix powder composites reinforced by nanoinclusions of ZrO_2

We consider metal–matrix powder composites reinforced by nanoinclusions of ZrO_2. In order to create such a composite material, aluminium powder with a specific surface of 0.58 m^2/g, with spherical shape particles, whose diameter is not more than 20 μm was used. As reinforcing particles, we used nanopowders of stabilized zirconium oxide that are synthesized in plasma (see Fig. 1). The specific surface of nanopowders ranged from 18 to 32 m^2/g, which corresponds to an average particle diameter $d = 58 - 33$ nm. It is believed that the initial nanoparticles are spherical in shape. Larger particles have both spherical and irregularly shapes. Irregular particles are sintered aggregates of primary nanoparticles.

By pressing, we obtained test samples of composite material with a volume content of nanopowders of 0.01%, 0.05%, 0.1% and 0.15%. The samples are in cylindrical form. Pressing force for all samples was 400 MPa. Sintering of samples was conducted in a vacuum for 240 min at a temperature of 640 °C.

To determine the pycnometric density of receiving samples, we used helium pycnometer Ultrapycnometer 1200e. The structure of the composite sample was studied on scanning electron microscope FEI Quanta 600 FEG and inverted metallographic microscope Carl Zeiss Axiovert 40 MAT. Testing the compressive strength was carried out on a universal machine for mechanical testing LF-100 K (Walter + Bai).

The results of studies of the structural and mechanical properties of the samples are presented in Table 1.

It was found that when the volume fraction of nanoinclusion changes, a typical size of a grain of the aluminium matrix also changes. Moreover, there is a non-monotonic dependence of the