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VIII ВСЕРОССИЙСКАЯ НАУЧНО-ПРАКТИЧЕСКАЯ КОНФЕРЕНЦИЯ С МЕЖДУНАРОДНЫМ УЧАСТИЕМ, ПОСВЯЩЕННАЯ 50-ЛЕТИЮ ОСНОВАНИЯ ИНСТИТУТА ХИМИИ НЕФТИ

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MULTISCALE MODELING THE MECHANICAL BEHAVIOR OF BIOINERT Ti-Nb ALLOYS

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The aim of the work was to develop a multi-scale computational model for predicting the mechanical properties of bioinert ultrafine-grained (UFG) Ti-Nb alloys with high specific strength, lower elastic moduli to replace full-scale experimental studies with computer simulation of promising and developed alloys with regard to structure at different scale levels.

The predictions of the mechanical properties of Ti-Nb alloys were obtained using the results of simulation the response of model volumes of single-phase and multi-phase media to external thermomechanical effects. Model volumes of Ti-Nb alloys were created taking into account the data on the distribution of phases obtained as a result of microstructural studies of experimental samples of the alloys. It was taken into account that the volume concentrations of alpha, alpha’’ and beta phases in the structure of Ti-Nb depend on the concentration of Nb and the heat treatment regimes. The plastic flow of alpha and beta phases was described using variants of microdynamic constitutive equations for metals with a face-centered cubic lattice (for the alpha phase) and a body-centered lattice (for the beta phase). It was shown that UFG Ti-Nb alloys exhibit higher values of the yield strength, but significantly lower values of strain hardening as compared to coarse grained alloys.

The effective shear stresses are calculated by the algebraic sum of the stresses from the external load and the components of the back stresses. The components of internal back stresses are calculated by the sum of the components depending on the accumulated density of dislocations, the Orowan stresses arising around the nano-size inclusions, as well as the stress components caused by the twins substructure and grain boundaries.

The increment of plastic strain caused by a twinning in Ti-Nb alloys is determined by a semi-phenomenological equation. This equation relates the increment of shear plastic deformation with the increment of the volume concentration of twins and the displacement of the crystal lattice during twinning:

We simulated the response of the model volume of single-phase and multi-phase media to external thermomechanical effects for prediction of Ti-Nb mechanical behavior. The simulation of the effects of pulses on the boundary of the model volume made it possible to calculate the propagation velocity of elastic waves and determine the effective elastic moduli for multiphase alloys without invoking additional hypotheses about the effect of the structure on the elastic properties of Ti-Nb alloys.

The anisotropy effect of the elastic properties of the grains can be neglected due to the small effect on the average stress components in the representative volume of ultrafine-grained alloys or alloys with a bimodal grain size distribution compared to the anisotropy effects resulting from plastic deformation.

The developed multilevel model allows using the results of modeling the propagation of stress waves in model volumes of alloys to predict the magnitude of the elastic moduli of Ti-Nb alloys taking into account the phase composition of the alloys and the grain size distribution.

It was shown that the dependence of the Young's modulus of Ti-Nb alloys on the concentration of Nb in the range from 1 % to 45 % by weight is non-monotonic. Stress-strain curves of Ti-Nb alloys under tension were obtained by computer simulation. Model volumes of coarse-grained and ultrafine-grained Ti-Nb alloys with Nb concentrations of 1%, 13% and 45% were simulated at strain rate of 0.01 s^{-1} at 295 K. Calculated stress-strain curves are shown in Fig.1. The Ti – 13Nb-13Zr alloy consisted of grains of a solid Nb solution in the alpha phase of Ti, a solid solution of Nb in the beta phase of Ti, and particles of Nb in the beta phase.

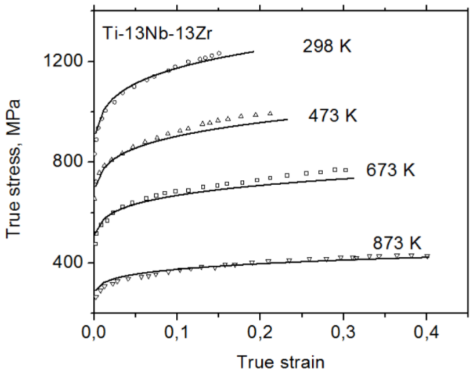

Fig. 1. Calculated stress-strain curves of coarse-grained Ti – 13Nb-13Zr alloy under tension. Symbols are experimental data [1]

Stress-strain curves of coarse-grained (1) and ultrafine-grained (2) Ti – 45Nb alloy under tension are shown in Fig.2.

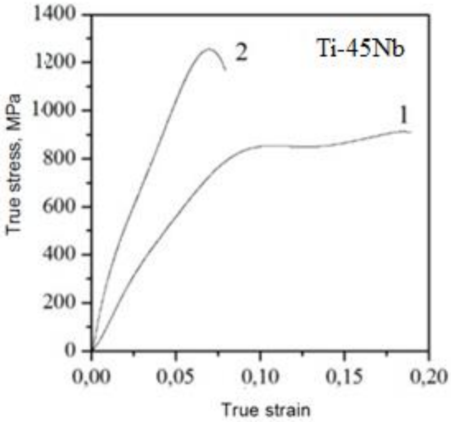

Fig. 2. Stress-strain curves of coarse-grained (1) and ultrafine-grained (2) Ti – 45Nb alloy under tension [2]

It was shown that Ti-Nb alloys with ultrafine-grained structure exhibit higher values of yield strength, but significantly lower values of strain hardening as compared to alloys in the large-crystalline state. Mechanical response of model volumes of Ti-Nb alloys was simulated in the range of temperature variation from 295 K to 873 K, taking into account changes in thermally activated dislocation mechanisms of plastic deformation and twinning [3]. It was shown that an increase in temperature in the specified range leads to a decrease in the yield strength and flow stress of the Ti-13% Nb alloy by three times.

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