Study of hardening mechanisms, residual stresses and microstructure of high-strength aluminum alloys

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The presented series of papers is devoted to the study of high-strength aluminum alloys, which are widely used in many industries due to their high mechanical strength and low weight. However, often at temperatures above 200 °C their mechanical properties deteriorate due to an increase in the creep process, in which the material slowly deforms under the influence of a constant load at elevated temperatures. Basically, material creep is caused by two factors: diffusion of atoms, leading to the formation of defects in the crystal lattice, and thermal activation of dislocations, facilitating their easier movement in the crystal lattice. Therefore, material creep can lead to a decrease in the strength and deformation of structures, as well as a decrease in resistance to destruction under long-term loading.

Various methods are used to solve the problem of creep in high-strength aluminum alloys. One of them is the addition of alloying elements that lead to the formation of dispersed particles of secondary phases (carbides, nitrides, etc.), which helps to strengthen the material and increases the resistance of the alloy to creep. Another method is special heat treatments that can lead to a change in the size and shape of the grain, which helps to stabilize the dislocation structure of the alloy and limits the movement of dislocations, and thereby reduces the tendency of the material to creep. However, the problem of creep in high-strength aluminum alloys is still the subject of active research around the world, aimed at developing new alloys and technological processes to increase the strength and stability of these materials. Improving the strength characteristics of aluminum alloys at elevated temperatures will eventually allow replacing more expensive light alloys (for example, titanium or magnesium) in industrial products. In this regard, a special subject of interest is the study of the creep mechanisms of aluminum alloys at different temperatures and the mechanisms of strengthening depending on heat treatment, as well as the distribution of residual macro- and microstresses in industrial products made of these materials, which is fully reflected in the subject matter of the presented cycle of works.

In papers [1-2], two series of aluminum alloy powders of commercial grades 2014Al and 2124Al with different durations of aging heat treatment were studied. Based on the results of studies using complementary experimental methods, including scanning electron microscopy (SEM), neutron and X-ray diffraction, and small-angle neutron scattering (SANS), it was found that in addition to the main phase of aluminum, these alloys contain nanosized dispersed particles of secondary phases (precipitates). Data were obtained on the evolution of precipitate phases, as well as other microstructure parameters of the studied alloys (crystal lattice parameters, microstrains, particle sizes, phase content) depending on the duration of heat treatment. Based on these data, model calculations were made that made it possible to estimate the strengthening contributions from solid solution atoms and precipitates in the creep

equation for 2014Al and 2124Al aluminum alloys, linking the normalized strain ε with the normalized stress σ, and, thus, to describe the behavior of these materials under creep deformation.

Another important factor that significantly affects the creep behavior of aluminum alloys is the configuration of the dislocation structure in the material. In [3], the deformation behavior of two materials (pure aluminum Al-99.8% and Al-3.85%Mg alloy), which have very different creep characteristics, was studied using neutron diffraction and backscattered electron diffraction (EBSD). In the case of aluminum Al-99.8%, a subgrain structure is formed during creep, and in the case of the Al-Mg alloy, dislocation forests (structures of uniformly distributed dislocations) are formed. Comparison of neutron diffraction and EBSD-KAM data allowed us to draw conclusions about the correlation between the dislocation substructures generated during creep, microstrain and crystal orientation inherited from the extrusion process, which leads to different behavior of the materials during creep deformation.

A very important aspect for the industrial application of high-strength aluminum alloys is the study of the stress-strain state in products made of these materials. Usually, as a result of mechanical or thermal treatment, as well as under external loading, residual stresses of the 1st kind (macrostresses) arise in the sample material, which are quite easily determined using diffraction methods. Macrostresses are approximately uniform in magnitude and direction over macroscopic scales in the material that exceed the sizes of several grains and are balanced over the whole volume of the sample. In works [4-5], the distribution of residual macrostresses in cylindrical samples of 5083Al and 2014Al aluminum alloys subjected to quenching and annealing was studied using the neutron diffraction method. It was shown that in quenched cylindrical samples, a parabolic profile of the distribution of residual macrostresses arises, inherited from the extrusion process [4]. In this case, the maximum value of residual stress in the quenched sample of the age-hardened alloy 2014Al is almost 2 times lower than in the non-aging alloy 5083Al. This difference is completely consistent with the results of work [5], in which, based on numerical calculations by finite element method (FEM), it was established that the level of residual macrostresses depends not only on the thermal and mechanical properties of the alloys, but also on the parameters of strain hardening of the material and the dimensions (diameters) of the cylindrical samples.

In addition, based on the analysis of the shape of the diffraction peaks, it was assumed that there are significant residual stresses of the 2nd kind (homogeneous microstresses) in the studied alloys due to heat treatment. These microstresses are approximately uniform in magnitude and direction over microscopic scales in the material and are balanced within one grain. Residual microstresses often arise due to unequal elastic properties and yield strength in individual grains of the material, so their determination is a highly non-trivial task. Adequate assessment of the level of residual microstresses in the material is of great importance for the optimization of technological processes, since they can be the cause of fatigue damage and corrosion cracking of structures.

To solve this problem, an original method for calculating residual microstresses in a hardened cylindrical sample of extruded single-phase alloy 5083Al is proposed in [6-8]. The calculations were performed using a genetic algorithm (GA), which is a method for solving optimization problems based on the biological principle of natural selection and is one of the varieties of the method of evolutionary calculations - a direction in the class of artificial intelligence (AI) methods. The input data for the GA algorithm are the profiles of neutron diffraction peaks from crystallites with a certain orientation <hkl>, measured on a neutron Fourier stress diffractometer FSD at the IBR-2 reactor in the FLNP JINR, and the microstructure parameters obtained by the electron backscatter diffraction (EBSD) method. The GA algorithm assigns a stress value to each crystallite in accordance with the diffraction peak profiles and

microstructural parameters of the crystallites. Using GA, the problem of symbolic regression was solved, during which a search was made for a mathematical function describing the dependence on microstructural parameters: $d_{hkl}^{n} = d_{hkl}^{n}(A_n, I_n, AR_n, S_n)$, where A_n is the crystallite area, I_n is the number of neighboring crystallites, AR_n is the aspect ratio of the crystallite, S_n is the slope of the crystallite or, tan(θ), where θ is the angle between the direction of the long axis of the crystallite and the radial axis of the sample, n is the crystallite number from all measured EBSD. In [6], the GA method was used to find the best acceptable expression for $d_{hkl}^{n}(A_n, I_n, AR_n, S_n)$, among a mathematical tree of all possible solutions, which completely reproduces the profile of the (111) diffraction peak and predicts the value for each crystallite n with the <111> orientation. From this information, lattice strains and total stresses were calculated for all crystallites using Young's modulus for the <111> orientation. Next, the values of residual microstresses were calculated as the difference between the total and macroscopic stress for each crystallite n with the <111> orientation. Thus, as a result of calculations using the GA method, a map of residual microstresses was constructed for crystallites with the <111> orientation. A more complete study based on data measured at various points of the sample, and in which families of crystallites <111>, <200>, <220>, <311> are considered, is presented in [7]. Also in work [8], using the example of a hardened cylindrical sample made of non-aging 5083Al alloy, the advantage of a combined approach based on the stress balance method and GA for determining the undeformed lattice parameter d_0 is shown in comparison with the processing of individual diffraction peaks or the entire spectrum as a whole according to the Rietveld method.

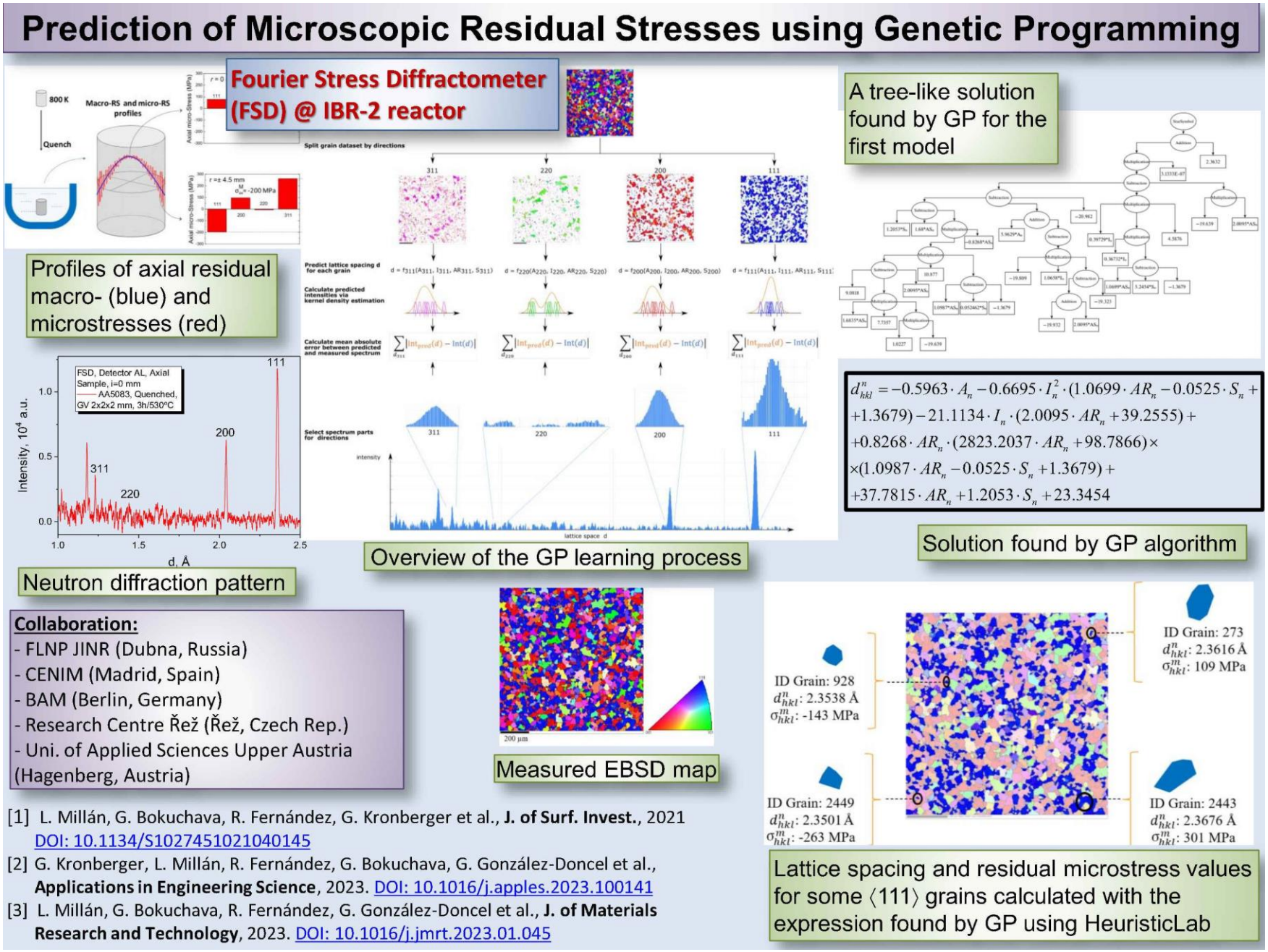
Thus, the performed experiments have shown that the unique technique - neutron correlation time-of-flight Fourier diffractometry, used on the Fourier stress diffractometer FSD at the IBR-2 reactor, allows achieving high sensitivity of the instrument and provides precision measurement of residual strains and microstrains in the study of modern structural materials. The combined use of high-resolution neutron diffraction and other experimental methods made it possible to use modern approaches to data processing using artificial intelligence (AI) methods to successfully solve a number of complex problems of materials science devoted to the problem of creep and residual (micro)stresses in high-strength aluminum alloys.

The studies of high-strength aluminum alloys were carried out by the staff of the FLNP JINR in an international collaboration with the National Center for Metallurgical Research (CENIM, CSIC) (Madrid, Spain), the Federal Institute for Materials Research and Testing (BAM) (Berlin, Germany), the Research Center Řež (Řež, Czech Republic), the Laboratory of Heuristic and Evolutionary Algorithms of the Upper Austrian University of Applied Sciences (Hagenberg, Austria), and the Complutense University of Madrid (Madrid, Spain).

The papers of the presented series were published in highly ranked journals, including Journal of Alloys and Compounds (IF = 6.371), Journal of Materials Research and Technology (IF = 6.267), Journal of Applied Crystallography (IF = 6.10) and Advanced Engineering Materials (IF = 2.906).

List of publications

1. G. Bokuchava, Yu. Gorshkova, R. Fernández, G. González-Doncel, G. Bruno, Characterization of precipitation in 2000 series aluminium alloys using neutron diffraction, SANS and SEM methods, Romanian Reports in Physics, 2019, Vol. 71, No. 1, Article No. 502, pp. 1-12. Q2 IF 1.940 https://rrp.nipne.ro/2019/AN71502.pdf
2. R. Fernández, G. Bokuchava, I. Toda-Caraballo, G. Bruno, V. Turchenko, Yu. Gorshkova, G. González-Doncel, Analysis of the combined strengthening effect of solute atoms and precipitates on creep of aluminum alloys, Advanced Engineering Materials, 2020, Vol. 22, 1901355. Q1 IF 2.906 https://doi.org/10.1002/adem.201901355
3. R. Fernández, G. Bokuchava, G. Bruno, I. Serrano-Muñoz, G. González-Doncel, On the dependence of creep on the crystal orientation in pure Al and Al-Mg, Journal of Applied Crystallography, 2023, Vol. 56, pp. 764-775. Q1 IF 6.10 https://doi.org/10.1107/S1600576723003771
4. L. Millán, G. Bokuchava, R. Fernández, I. Papushkin, G. González-Doncel, Further insights on the stress equilibrium method to investigate macroscopic residual stress fields: case of aluminum alloys cylinders, Journal of Alloys and Compounds, 2021, Vol. 861, 158506. Q1 IF 6.371 https://doi.org/10.1016/j.jallcom.2020.158506
5. G. Carro-Sevillano, R. Fernández, G. Bokuchava, L. Millán, G. González-Doncel, Residual stress distribution after quenching treatment obtained from diffraction experiments and simulation by finite element method, Journal of Surface Investigation. X-ray, Synchrotron and Neutron Techniques, 2021, Vol. 15, No. 3, pp. 537-541. Q3 IF 0.359 https://doi.org/10.1134/S1027451021030071
6. L. Millán, G. Bokuchava, J.I. Hidalgo, R. Fernández, G. Kronberger, P. Halodova, A. Sáez, I. Papushkin, O. Garnica, J. Lanchares, G. González-Doncel, Study of microscopic residual stresses in an extruded aluminium alloy sample after thermal treatment, Journal of Surface Investigation. X-ray, Synchrotron and Neutron Techniques, 2021, Vol. 15, No. 4, pp.763-767. Q3 IF 0.359 https://doi.org/10.1134/S1027451021040145
7. L. Millán, G. Kronberger, R. Fernández, G. Bokuchava, P. Halodova, A. Sáez-Maderuelo, G. González-Doncel, I.J. Hidalgo, Prediction of Microscopic Residual Stresses using Genetic Programming, Applications in Engineering Science (Open access journal), 2023, Vol. 15, 100141. Q2 CiteScore 2.1 https://doi.org/10.1016/j.apples.2023.100141
8. L. Millán-García, G. Bokuchava, P. Halodova, A. Sáez-Maderuelo, G. González-Doncel, J.I. Hidalgo, J.M. Velasco, R. Fernández, Using genetic programing and the stress equilibrium method to obtain the un-stressed lattice parameter for calculating residual stresses, Journal of Materials Research and Technology, 2023, Vol. 23, pp. 1543-1558. Q1 IF 6.267 https://doi.org/10.1016/j.jmrt.2023.01.045



$$d^n_{hkl} = -0.5963 \cdot A_n - 0.6695 \cdot I_n^2 \cdot (1.0699 \cdot AR_n - 0.0525 \cdot S_n + \\ +1.3679) - 21.1134 \cdot I_n \cdot (2.0095 \cdot AR_n + 39.2555) + \\ +0.8268 \cdot AR_n \cdot (2823.2037 \cdot AR_n + 98.7866) \times \\ \times (1.0987 \cdot AR_n - 0.0525 \cdot S_n + 1.3679) + \\ +37.7815 \cdot AR_n + 1.2053 \cdot S_n + 23.3454$$

[1] L. Millán, G. Bokuchava, R. Fernández, G. Kronberger et al., **J. of Surf. Invest.**, 2021 DOI: 10.1134/S1027451021040145

[2] G. Kronberger, L. Millán, R. Fernández, G. Bokuchava, G. González-Doncel et al., **Applications in Engineering Science**, 2023. DOI: 10.1016/j.apples.2023.100141

[3] L. Millán, G. Bokuchava, R. Fernández, G. González-Doncel et al., **J. of Materials Research and Technology**, 2023. DOI: 10.1016/j.jmrt.2023.01.045

Fig. 1. Scheme for calculating the residual microstress map using a genetic algorithm (GA) based on experimental data from neutron diffraction (Fourier stress diffractometer FSD at the IBR-2 reactor) and electron backscatter diffraction (EBSD).