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Methodological aspects of training dataset construction for predicting the mechanical strength of filled polymer coatings during natural climatic aging

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Abstract. The paper presents the results of investigating the strength characteristics of eleven compositions of protective and decorative epoxy polymer coatings with mineral fillers and an unfilled polymer under natural climatic aging in a temperate climate (Saransk). The work formalises the methodological approach to the formation of a training dataset for predicting changes in the strength characteristics of polymer composites with mineral fillers using machine learning methods. It is shown that with the introduction of a mineral filler, the failure mode of the epoxy matrix under bending changes from viscous-fluid to brittle, which allows the bending strength to be unambiguously determined. Under uniaxial compression, the classical strength value is reached in the region of relative strains of 50 % and higher, which corresponds to the densification phase of the already failed material and does not physically reflect the actual strength response. As a methodologically correct alternative, the yield strength is proposed, identified as the first local maximum on the smoothed σ–ε curve and unambiguously determined for all studied compositions at all natural climatic aging points. The relative difference Δσ between the strength value (in bending) or the yield strength (in compression) of the filled composition and the corresponding stress value on the deformation curve of the unfilled polymer, taken at the same point of relative strains for each time point of climatic aging, is proposed as the target feature of the prediction model. This approach automatically eliminates from the target variable the components associated with the post-curing effects and the degradation of the polymer matrix itself, leaving the model with the task of predicting the contribution of the filler and the state of the polymer–filler interface. Based on the analysis of the reinforcing effect of the eleven filled compositions in the reference state without post-curing, three groups of fillers are identified according to the level of the relative strength gain under bending («low» 3÷10 %, «moderate» 24÷53 %, «high» 70÷120 %), which are consistent with the physical picture of the filler–polymer matrix interaction. Recommendations are formulated on the composition of the model's input feature space, including the type and shape of the filler particles, the mass fraction, the characteristic particle size, the specific surface area, and the characteristic relative strain of the composition in the reference state. It is noted that the bending tests possess substantially greater informativeness in the assessment of the climatic resistance of the investigated class of materials in comparison with uniaxial compression.
Keywords: epoxy polymer composites, mineral fillers, natural climatic aging, bending strength, yield strength in compression, reference curve, machine learning, training dataset

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1. INTRODUCTION

Protective and decorative polymer coatings based on epoxy resins with dispersed mineral fillers are widely used in construction practice for protecting concrete, metal, and wooden substrates against aggressive environments [1, 2]. The introduction of mineral fillers into the polymer matrix is motivated by a complex set of technological and operational factors – reducing the cost of the protective coating through the partial replacement of the expensive polymer binder with a cheaper mineral phase, the targeted control of the technological characteristics of the uncured composition, as well as the modification of the physical-mechanical, thermophysical and other service properties of the final coating [3]. Along with this, the very fact of introducing a mineral filler fundamentally changes the behaviour of the material under the action of aggressive environments by forming additional pathways of environmental penetration into the bulk of the material at the «polymer matrix – filler» interface, with subsequent initiation and development of microdamage and accumulation of irreversible changes during service, which ultimately determines the residual operational load-bearing capacity of the coating [4–6]. Considering that climatic action represents the most widespread aggressive environment – particularly for epoxy polymers, which form a typical base of many protective and decorative coatings with mineral fillers – the task of predicting their residual service life under climatic aging represents an urgent problem [7–9].

The modern approach to predicting the residual service life of a number of materials under natural operating conditions is based on the application of machine learning methods, which make it possible to establish quantitative relationships between the integral indicators of climatic action and the characteristics of the current state of the material [10–12]. As applied to polymer protective and decorative coatings with dispersed mineral fillers, machine learning makes it possible to simultaneously solve two methodological tasks – to quantitatively describe the combined response of the material to a complex multi-factor climatic regime, and to systematically isolate the contribution of the chemical nature, particle size distribution and particle shape of the mineral filler to the overall degradation kinetics. The quality of the machine learning model prediction, however, fundamentally depends on the composition and structure of the training dataset – on the volume of experimental data, the choice of target feature, the input feature space and the model validation strategy [13], which places the task of methodological formalisation of the training dataset preparation among the priority issues in the development of prediction models based on natural climatic test results.

The strength characteristics of protective and decorative epoxy coatings belong to the group of indicators determined by destructive methods, which establishes peculiarities of their existence in the space of target features. On the one hand, the values of the ultimate strength under bending and compression directly characterise the residual operational load-bearing capacity of the coating, which makes them a key indicator for the assessment of filled polymer composites. On the other hand, the destructive character of the test does not allow obtaining the characteristic values of the property changes of the material within a single specimen – every test results in its destruction, which requires a fundamentally different approach to the formation of the training dataset compared with the indicators obtained by non-destructive methods. In addition, the very notion of «ultimate strength» for the studied class of materials turns out to be methodologically ambiguous – the transition from a viscous-fluid to a brittle failure mode upon the introduction of a mineral filler, together with the substantial difference in the shape of the σ–ε curves under bending and compression, form an independent task of selecting a physically relevant and unambiguously defined characteristic point for strength assessment, consistent both between the studied compositions and between various durations of natural climatic exposure.

The aim of the present work is to formalise the methodological approach to the formation of a training dataset for predicting changes in the mechanical strength of epoxy polymer coatings with dispersed mineral fillers under natural climatic aging, including the justification of the choice of a quantitative strength metric for the two regimes of destructive loading (three-point bending and uniaxial compression), the identification and justification of the appropriateness of using particular target features of the models, as well as the formulation of recommendations on the construction of the input feature space consistent with the physical picture of the filler–polymer matrix interaction under natural exposure.

2. METHODS AND MATERIALS

To evaluate the changes in the mechanical strength, plate-shaped specimens with dimensions of 120×120×20 mm were manufactured without additional thermal treatment (post-curing) and subsequently placed onto the test stands. From the produced plates, two types of specimens were cut for testing – beams of 20×20×70 mm for three-point bending (with a support span of 60 mm) and cubes of 20×20×20 mm for uniaxial compression. For each composition at each measurement point, 6 beam specimens and 6 cube specimens were obtained, which ensures the reproducibility of the statistical assessment of the indicators. In the bending tests, the front (face) surface of the specimens was placed in the tensile zone, thereby ensuring the maximum sensitivity of the test to the changes occurring in the surface layers of the material during climatic aging. In compression, the cube specimens were tested in their design position (face upwards). The list of the studied compositions is given in Table 1.

Table 1. Coding and main characteristics of the studied protective and decorative coating compositions.

Composition code	Filler	Particle shape	Particle fraction / size	Mohs hardness	Filler content, wt. %
45M	–	–	–	–	–
051	Microcalcite (Elenin deposit)	cubic/cuboidal	0.5–1.0 mm	3	63.4
0205	Microcalcite (Elenin deposit)	cubic/cuboidal	0.2–0.5 mm	3	60.9
KM100	Microcalcite KoelgaCarb KM-100 (Elenin deposit)	cubic/cuboidal	d_{50} = 4.8 µm; d_{98} = 19.8 µm	3	51.1
AL3	Silanised aluminium hydroxide HDA MST-03	spherical	1.6–3 µm	3	42.8
AL50	Aluminium hydroxide TS 350	spherical	30–70 µm	3	45.0
T03	Silanised quartz sand T03	angular/irregular	~0.2–0.5 mm	7	57.6
KVM	Silanised quartz flour Beige	angular/irregular	< 50 µm	7	31.0
BARIUM	Barium sulphate (barite) Hosky	angular/irregular	d_{50} ≤ 1 µm	3.5	31.2
A20	Microtalc Talcon A-20	plate-like/flaky	d_{50} = 6 µm; d_max ≈ 20 µm	1	24.6
HOLLY	Calcined kaolin Holly 200	plate-like/flaky	d_{86} = 2 µm	2	28.1
KBCh	Kaolin KBCh-1	plate-like/flaky	up to 5 µm – 65 %; up to 20 µm – 90 %	2	28.3

The strength of the specimens was determined using a servo-hydraulic testing machine (type 13-DB/401) equipped with a climatic chamber (KPK 160 KH, controlled by GEOsys 8.7.8 software). The crosshead travel speed of the testing machine was 2 mm/min for bending tests and 4 mm/min for compression tests. The sampling interval for the load and displacement values was 0.01 s.

The values of the bending stress and the relative bending strain were calculated by the following formulas:

$$\sigma_{bend} = \frac{3 \cdot F \cdot L}{2 \cdot b \cdot h^2}, \tag{1}$$

where σ_{bend} – the bending stress, MPa; F is the load, N; L – the support span, mm; b – the mean width of the cross-section of the beam specimen (averaged over 3 measurements), mm; h – the mean height of the cross-section of the beam specimen (averaged over 3 measurements), mm;

$$\varepsilon_f = \frac{600 \cdot s \cdot h}{L^2}, \tag{2}$$

where ε_f – the relative bending strain, %; s – the deflection, mm; h – the specimen thickness, mm; L – the support span, mm.

The compressive stress was calculated using the formula:

$$\sigma_{comp} = \frac{F}{a \cdot b}, \tag{3}$$

where $\sigma_{сж}$ – the compressive stress, MPa; F – the load, N; a, b – the linear dimensions of the cross-section of the cube specimen, mm.

The methodology and calculation formulas for the three-point bending and uniaxial compression tests comply with the requirements of GOST 4648-2014 «Plastics. Method of testing for static bending» and GOST 4651-2014 «Plastics. Method of testing for compression», respectively.

3. RESULTS AND DISCUSSION

Typical shapes of the σ–ε curves for the bending and compression tests are shown in Fig. 1 and 2, respectively. The presented curves demonstrate a qualitatively similar structure for both loading regimes and differ only in the quantitative levels of the characteristic points. At the same time, the introduction of fillers, on average, leads to a decrease in the bending strength of the specimens and an increase in their compressive strength (Figs. 1, 2). The exception in terms of the failure mode in bending tests is the unfilled 45M composition, the specimens of which do not fail within the relative strain range of 0–10 %. This clearly indicates a change in the failure mode of the specimens under bending from viscous-fluid to brittle upon the introduction of mineral fillers at the filler contents selected within the framework of the present study. As a consequence, for the bending tests, the question naturally arises of choosing a relevant quantitative metric for evaluating the bending strength that allows the values to be compared both between specimens and between compositions. Fig. 3 presents a scatter plot of (ε, σ) combinations for the 11 filled compositions relative to the deformation curve of the unfilled 45M composition.

The mutual arrangement of the strength and relative strain values of the specimens under bending, shown in Fig. 3, indicates a fundamental feature of comparing the results of this type of test. The actual contribution of the filler to the change in the strength characteristics of beam specimens in bending tests should be assessed, on the one hand, on the basis of the change in the elastic response of the specimens up to the moment of failure, and, on the other hand, on the basis of the change in the deformability of the material due to filling. Young’s modulus in this case is a low-informative indicator, since it describes the behaviour of the material exclusively in the elastic range of relative strains (0.05–0.25 %). The results of the conducted studies have established that, for all fillers without exception, an increase or preservation of the bending strength compared with the unfilled 45M composition is observed at the relevant level of relative strains. The fillers can be grouped according to the degree of influence on the strength gain (the distance from the reference σ–ε curve of the unfilled 45M composition at the corresponding levels of relative strains): «low» (silica fillers KVM and T03, and microcalcite 051) – 3÷10 %; «moderate» (0205, AL3, BARIUM, A20, HOLLY) –

24÷53 %, and «high» – 70÷120 %. The identified grouping of fillers by the magnitude of the reinforcing effect is consistent with the physical picture of the filler-polymer matrix interaction. The greatest contribution to the strength gain is provided by fillers with a small characteristic particle size and high specific surface area, whereas fillers with a coarse fraction and low specific surface area give practically no difference between the unfilled material and the composite. The «moderate» group combines compositions with similar orders of magnitude of particle sizes but of different nature and particle shape. The obtained classification allows recommendations to be formulated regarding the feature space of the training dataset for the bending strength prediction model. As numerical features of the filler, along with the mass fraction of filler (Table 1), the characteristic particle size, specific surface area, and a categorical feature of particle shape are included in the initial sample. The stresses of the unfilled 45M polymer, measured at the value of relative strains at maximum load averaged for the given filler, serve as the reference level of the polymer matrix and are adopted as a correction value in the calculation of the model's target feature Δσ. Such an approach allows the contribution of polymer matrix degradation and the contribution of phase boundary degradation to the observed change in the strength of the filled composition during climatic aging to be quantitatively separated. Direct inclusion of the reference value $\sigma_o(\varepsilon_{ref})$ into the input feature set when the bending strength of the filled specimens after climatic aging σ_f is used as the target feature is limited by their strong interdependence, which with a small sample size will lead to a decrease in the generalisation ability of the model over the «filler – climatic aging conditions» combinations.

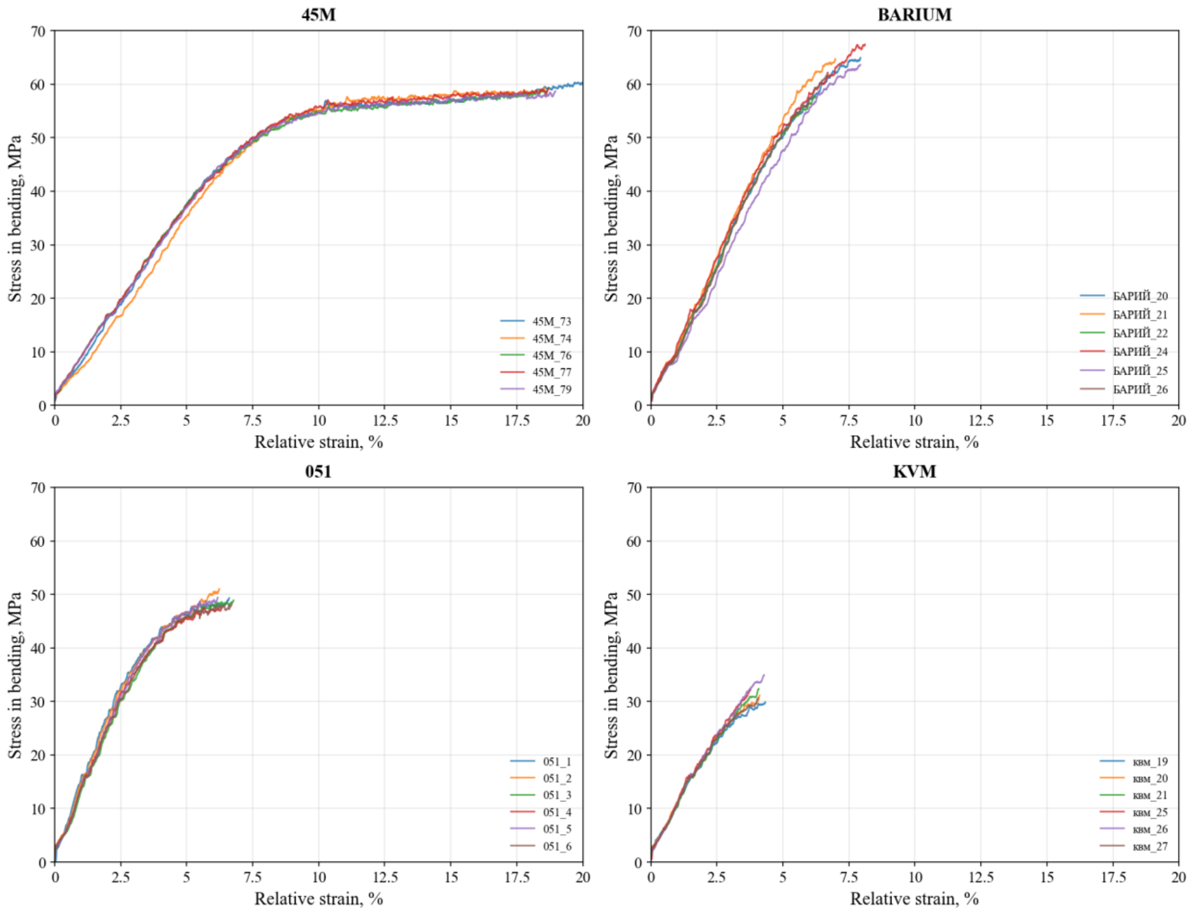

Fig. 1. Typical $\sigma - \varepsilon$ curves obtained in the bending tests of beam specimens.

When using Δσ as the model's target feature, for each of the filled compositions it is necessary to calculate the value of the individual characteristic relative strain per filled composition, with $\sigma_o(\varepsilon_{ref})$ computed at each measurement point on the basis of the values averaged over the studied specimens of the unfilled 45M polymer obtained after the corresponding duration of climatic aging. This will allow the degradation of the mechanical properties of the polymer matrix during climatic aging at each specific point to be accounted for, combined with the reliable quantitative isolation of the contribution of the phase boundary degradation. At the reference point, the results obtained for the unpost-cured 45M specimens should be used as reference values, due to the fact that the 120×120×20 mm plate specimens were placed onto the test stands without additional thermal treatment. The unfilled composition itself must be excluded from the training set in order to avoid double-counting of the reference level and the appearance of an incorrect class with zero levels of the features describing the filler used. An important advantage of this approach is the absence of the need to account for the stage of relaxation of the initial structural non-equilibrium, owing to the automatic subtraction of this effect when calculating the target feature $\Delta\sigma$.

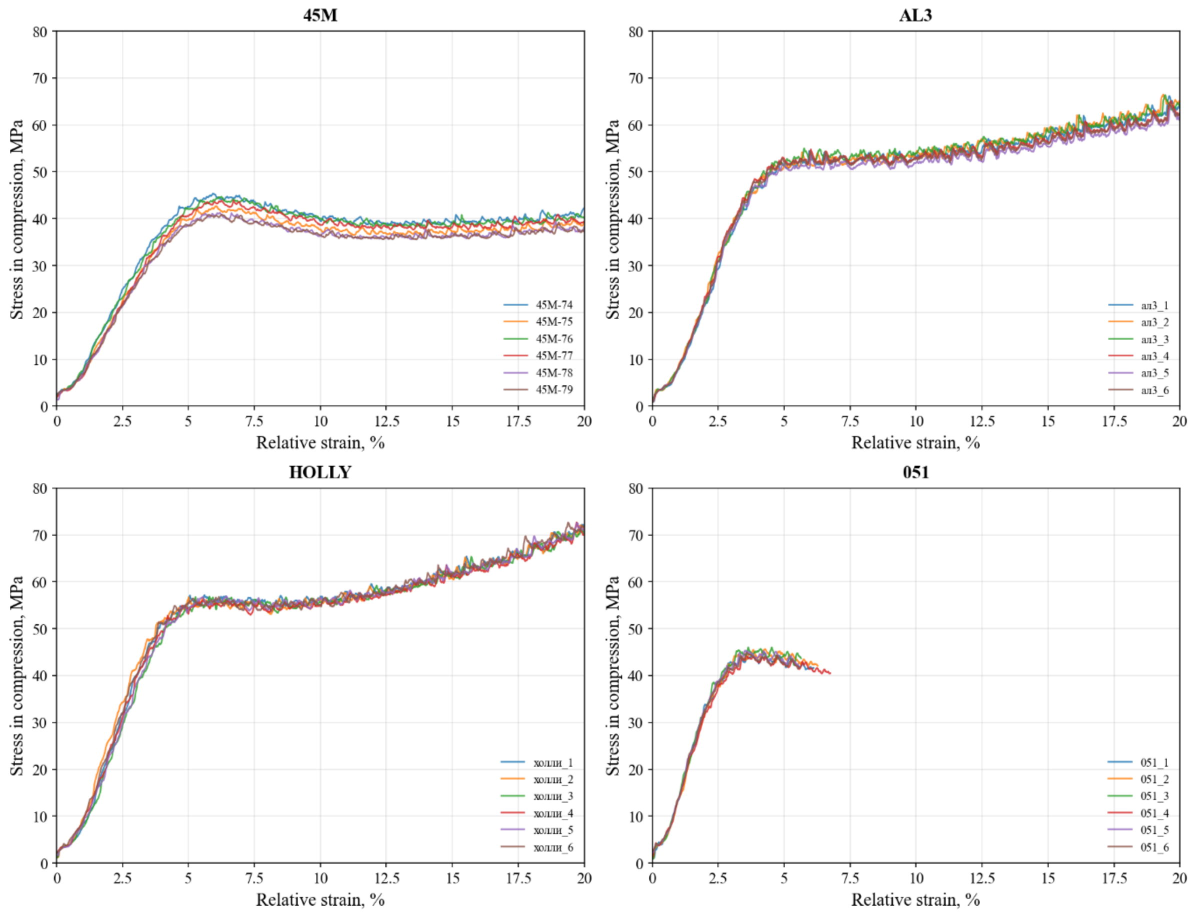

Fig. 2. Typical $\sigma - \varepsilon$ curves obtained in the compression tests of cube specimens.

Fig. 4 presents the evolution of the mechanical response of beam specimens of the unfilled 45M composition under bending during climatic aging. The qualitative shape of the curves is preserved for all points – a quasi-linear region up to the relative strain level of ≈ 5 % followed by a transition to a plateau. At the same time, the quantitative characteristics of the curves change significantly – an increase to ≈ 90 MPa after the first month of climatic aging followed by a decrease to ≈ 65 MPa by the fourth month, thereby reflecting the resulting ratio of the contributions of post-curing and degradation of the polymer matrix under the action of climatic factors. The qualitative coincidence of the shape of the curves of the specimens tested in parallel ensures the stability of the quantitative estimate of the mean response of the unfilled composition and allows the resulting smoothed curve, constructed from the averaged data, to be used as the reference curve at each time point.

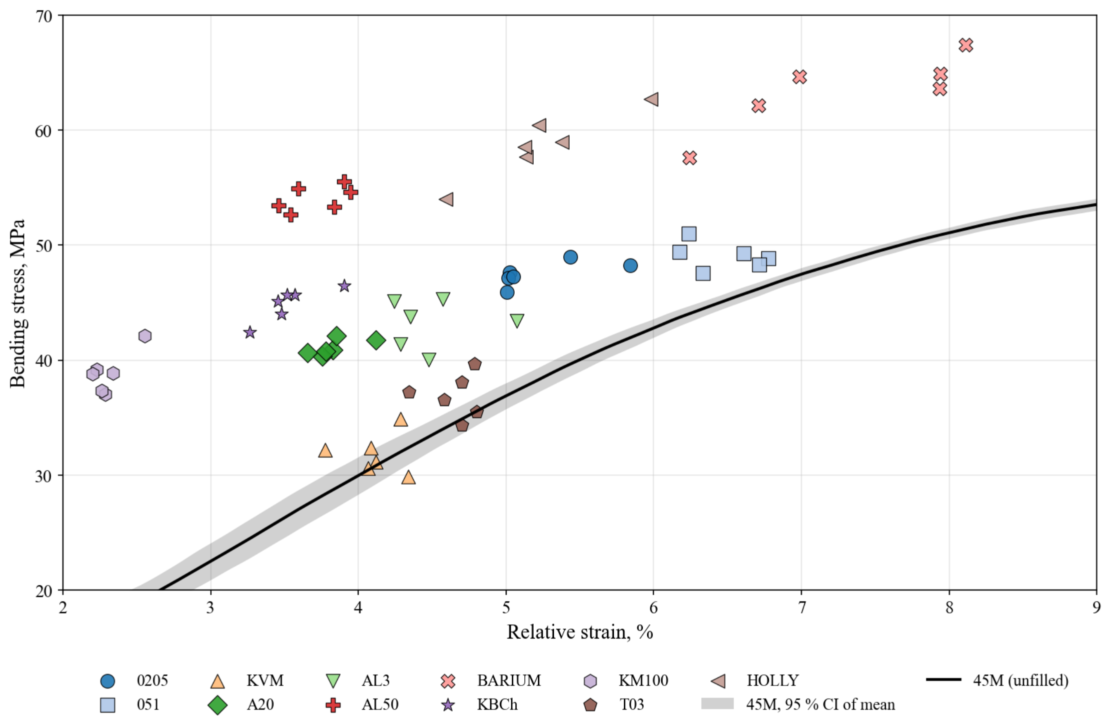

Fig. 3. Distribution of $\sigma_{bend} - \varepsilon_{max}$ values per specimen for the 11 filled compositions in the reference state under bend, supplemented by the smoothed average $\sigma - \varepsilon$ curve of the unfilled 45M composition with a 95 % confidence interval.

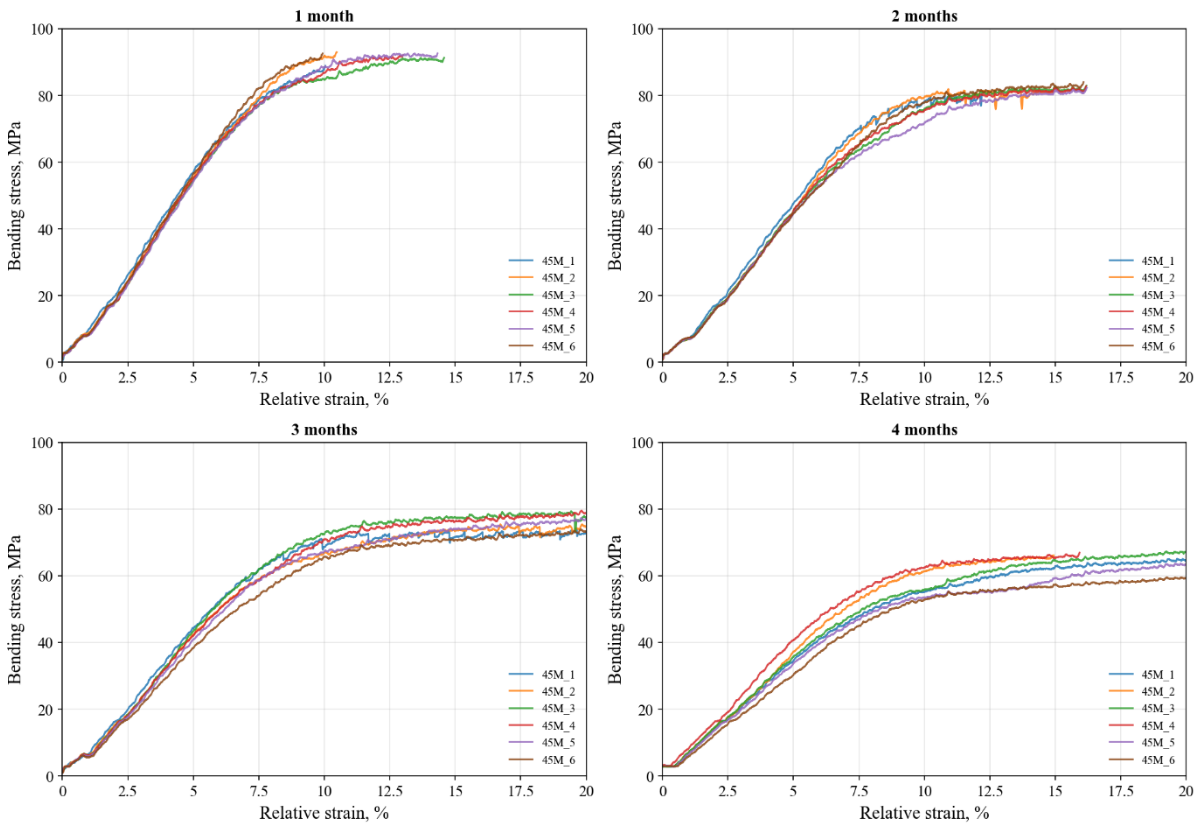

Fig. 4. $\sigma - \varepsilon$ curves of specimens of the unfilled 45M composition under bending loading as a function of the duration of natural climatic aging.

Fig. 5 shows the change in Δσ for the 11 filled compositions under study during climatic aging, calculated relative to the individual reference level at each measurement point and grouped according to the tentative division obtained for the unpost-cured state of the specimens at the reference point (Fig. 3). After an almost universally significant decrease in the gain relative to the reference value during the first month of climatic aging (clearly associated with the substantial increase in the absolute strength values for the 45M composition), all compositions except BARIUM and KBCh show either growth or preservation of the indicator above the initial level.

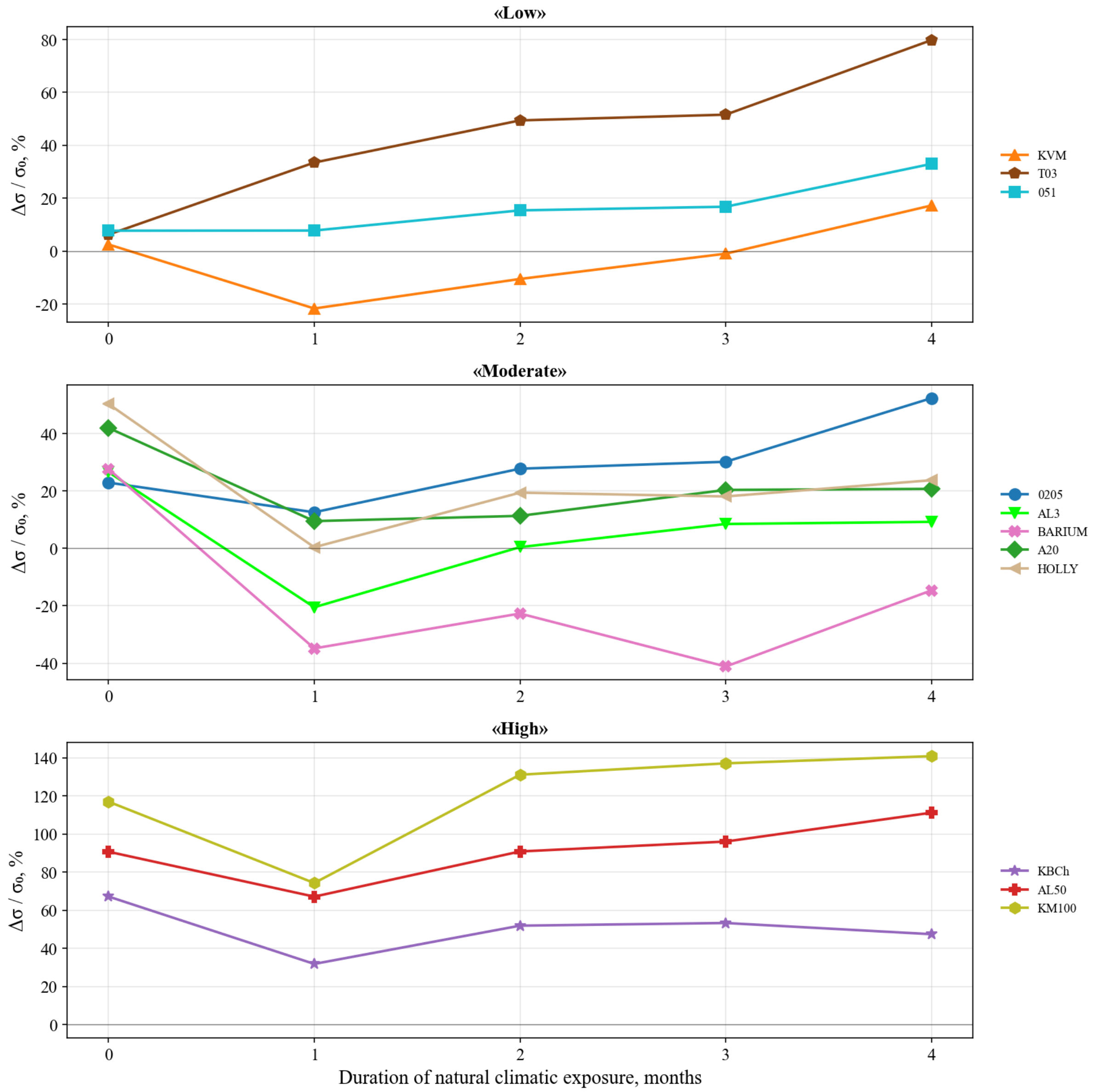

Fig. 5. Variation of the relative gain $\Delta\sigma$ of the specimens of the studied compositions in bending, calculated using the individual reference values for each measurement point, as a function of the duration of natural climatic aging.

The general growth trend of this metric for the vast majority of compositions is of fundamental importance for the machine learning problem statement – it indicates that the phase boundary degrades more slowly than the polymer matrix itself, which provides the physical possibility for independent prediction of the filler's contribution to the composite strength through the target feature Δσ.

Nevertheless, for the correct interpretation of the results, the gain function Δσ should be considered together with the absolute strength values for each of the studied compositions.

Figure 6 shows the absolute values of the bending strength of the specimens of the filled compositions, grouped by the magnitude of the reinforcing effect, in combination with the values obtained for the unfilled 45M composition (Fig. 3). The dynamics of a number of filled compositions qualitatively repeat the two-stage character of the kinetics of the polymer matrix itself: an increase in values during the 1st month of exposure relative to the starting state and a smooth decrease over the 2–4 month horizon. For the compositions of the «low» group and the AL50, KBCh, KM100 compositions of the «high» group, the absolute σ_f remains below the reference level of 45M throughout the entire exposure range, which, when analysed together with Fig. 5, indicates a substantial shift of the failure point towards smaller deformations while maintaining or slightly enhancing the response of the composite relative to the matrix. At the same time, it is important to note that the formal exceedance of the strength values of the 45M composition over those of the filled compositions at most time points is achieved at incomparably larger levels of the ultimate relative strains (ε ≈ 12–15 %, see Fig. 4). This fact further confirms the methodological limitation of using the bending strength σ_{max} and justifies the application of the metric Δσ at $\varepsilon = \varepsilon_{ref}$ as the target feature of the developed model.

The σ–ε curves of the compression tests of six cube specimens of four characteristic compositions in the reference state, shown in Fig. 2, reflect a fundamentally different behaviour of the material under load – after reaching a local maximum, generally identified as the yield strength of the material under compression σ_y, the curve transitions to a horizontal plateau followed by an accelerating rise, associated with strain hardening due to the densification of the failed material under conditions of limited volume.

A fundamental consequence of the obtained characteristic shape of the curve indicates the existence of a maximum strength value in the vicinity of relative strains of 50 % and higher, corresponding to the complete failure of the test specimen. Despite the multiple difference between σ_{max} and σ_y, real-world practice indicates the appropriateness of using the smaller value as the quantitative metric for evaluating the strength of the studied material in compression, primarily because the connectivity of the structure is preserved up to the level σ_y. However, the use of the designated σ_y metric as the target feature of the model requires a preliminary comparison with results methodologically identical to the bending test.

Figure 7 presents a diagram of the distribution of individual (ε, σ_y) values per specimen for the 11 filled compositions in the reference state without post-curing under compression, supplemented by the smoothed average σ–ε curve of the unfilled 45M composition with a 95 % confidence interval. The use of the yield strength σ_y as the quantitative strength metric under compression (Fig. 3) allows the range of characteristic deformations for all filled compositions to be obtained within a narrow band ε = 3.3–6.1 %, with all compositions located in the vicinity of the yield strength of the 45M composition. The points of ten out of eleven filled compositions are located above the reference 45M curve; the offset is 5–20 MPa depending on the composition, which indicates a lower relative effectiveness of the filler's influence on the level of the perceived load (9–26 MPa for bending). The cluster structure for the compression test results is less pronounced than for bending – only the KVM composition stands out as a separate group located below the reference 45M curve. Since the difference between compositions for the compression results is significantly less pronounced than for bending, the overall construction and analysis block will be carried out in accordance with the grouping previously obtained for bending (Fig. 3), thereby ensuring methodological continuity of data presentation and comparability between the two loading regimes.

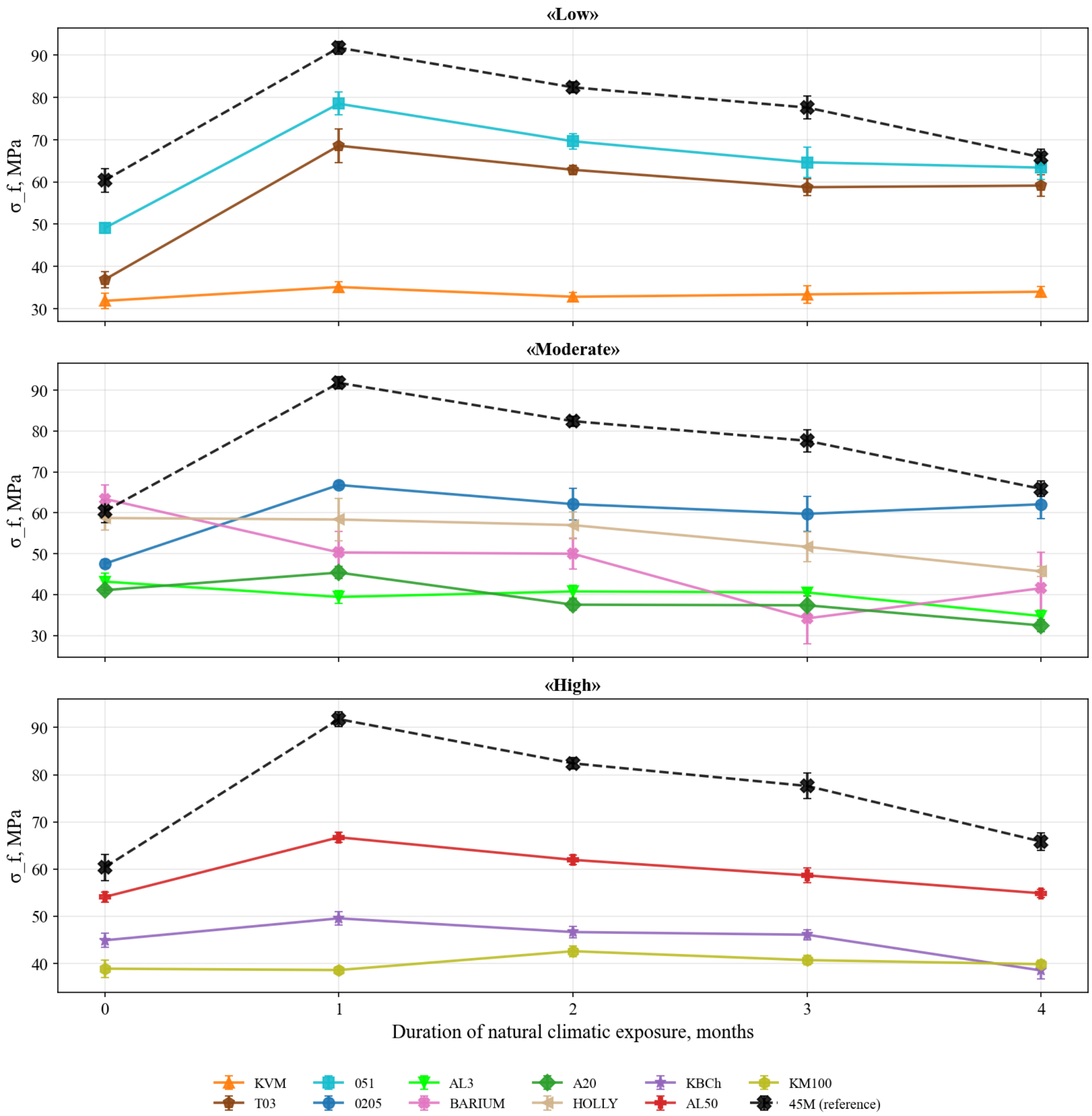

Fig. 6. Variation of the absolute values of the bending strength of the specimens of the studied compositions, grouped by the magnitude of the reinforcing effect $\Delta\sigma$.

Fig. 8 shows the σ–ε curves under compression of the cube specimens of the unfilled 45M polymer for the four climatic measurement points. The qualitative shape of the curves is preserved at all points and is consistent with the typical pattern of deformation of the epoxy matrix under compression with the transition to the yield strength in the vicinity of $\varepsilon \approx 5$ % followed by a horizontal plateau. The yield strength level increases to ≈ 70 MPa after the first month of climatic aging followed by a decrease to ≈ 50 MPa by the fourth month, which quantitatively coincides with the relative decrease in the bending strength of the same matrix (Fig. 4) – the common cause of the changes (the combination of post-curing with climatic aging) manifests itself in both loading regimes with a similar intensity of dynamics. The reproducibility between specimens tested in parallel is preserved at all points, which is confirmed by the spread of the peak yield strength values in the range of 4–5 MPa, which also indicates the correctness of using the smoothed 45M curve as the reference value when recalculating $\Delta\sigma$ of the filled compositions at each measurement point for the compression test results.

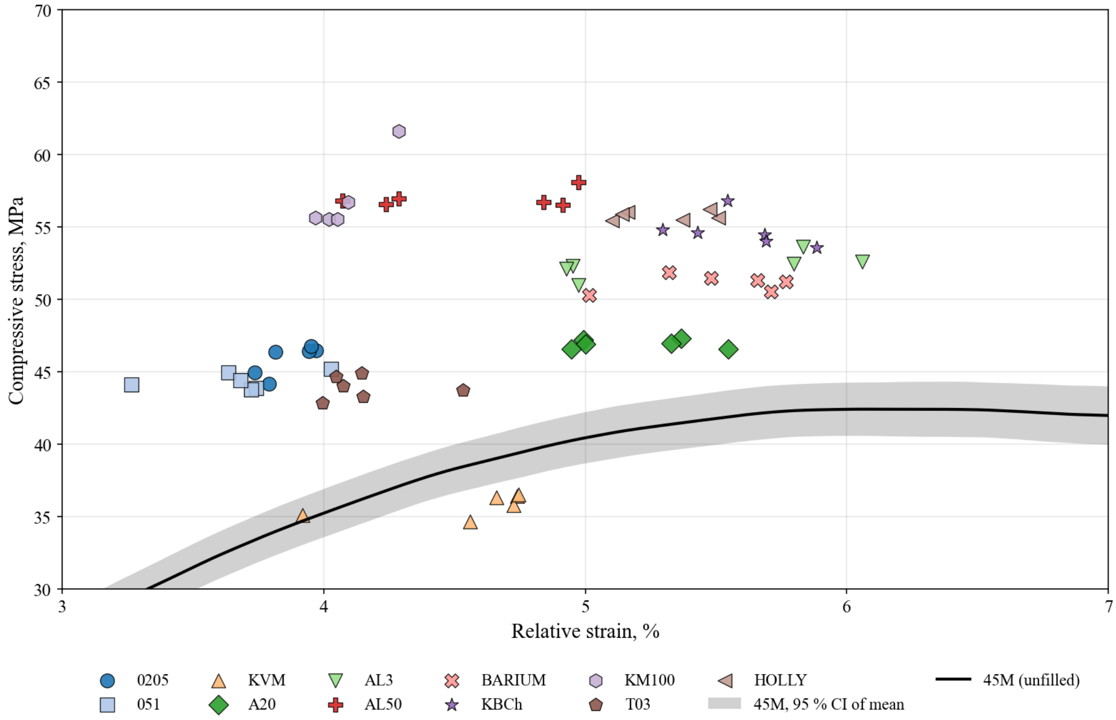

Fig. 7. Distribution of $\sigma_t - \varepsilon_{max}$ values per specimen for the 11 filled compositions in the reference state under compression, supplemented by the smoothed average $\sigma - \varepsilon$ curve of the unfilled 45M composition with a 95 % confidence interval.

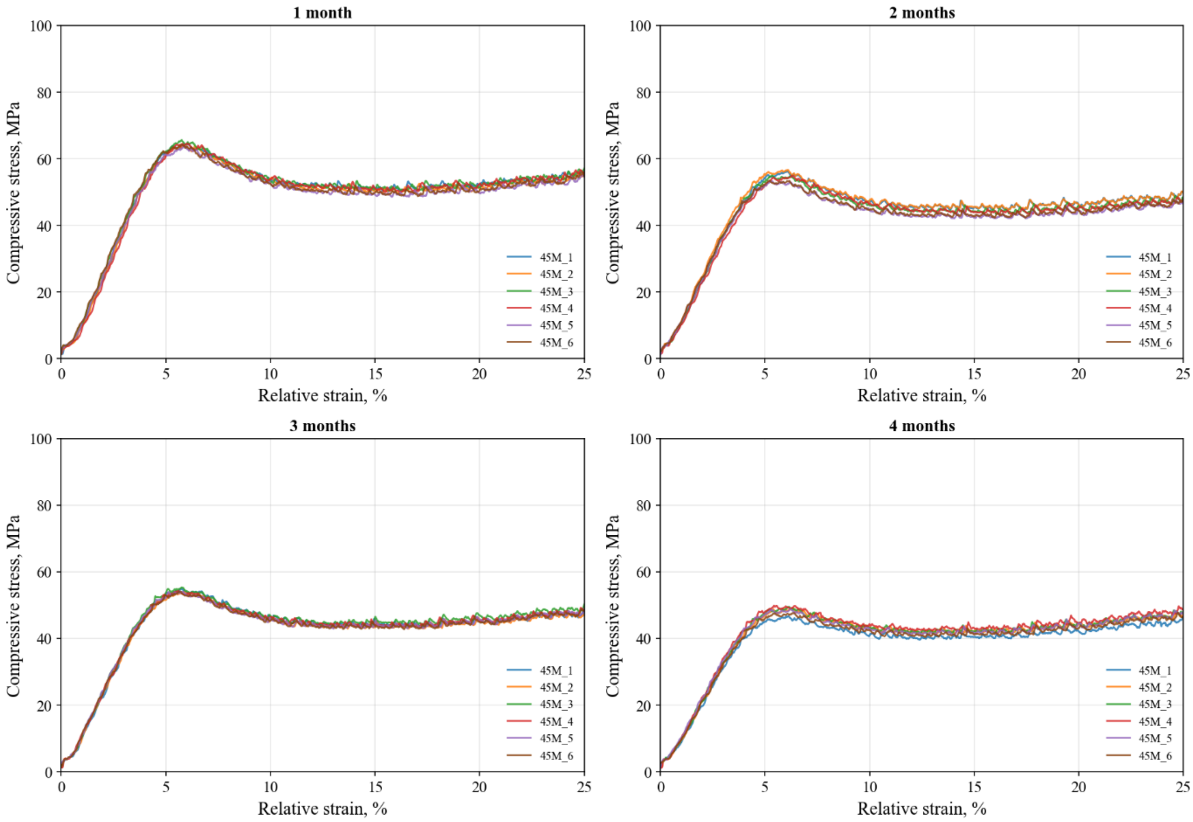

Fig. 8. $-\varepsilon$ curves of specimens of the unfilled 45M composition under compression loading as a function of the duration of natural climatic aging.

Fig. 9 presents the curves of the change of the relative gain Δσ for the compositions of the three groups (identical to those obtained earlier for the bending tests), calculated from the yield strength of the σ–ε curve of the filled composites and the values of the compressive stress of the unfilled 45M composition corresponding by relative strains. Unlike bending, in compression the absolute value of Δσ for most compositions and exposure points lies in the range of 10–60 %, which is several times lower than the corresponding values in bending – the reinforcing effect of the filler in compression is less pronounced and quantitatively manifests on a smaller scale. The dynamics observed for the compositions in compression depending on the group (Fig. 9) is consistent with that observed in bending (Fig. 5), which confirms the physical identity of the processes of post-curing and climatic degradation in filled composites in both loading regimes.

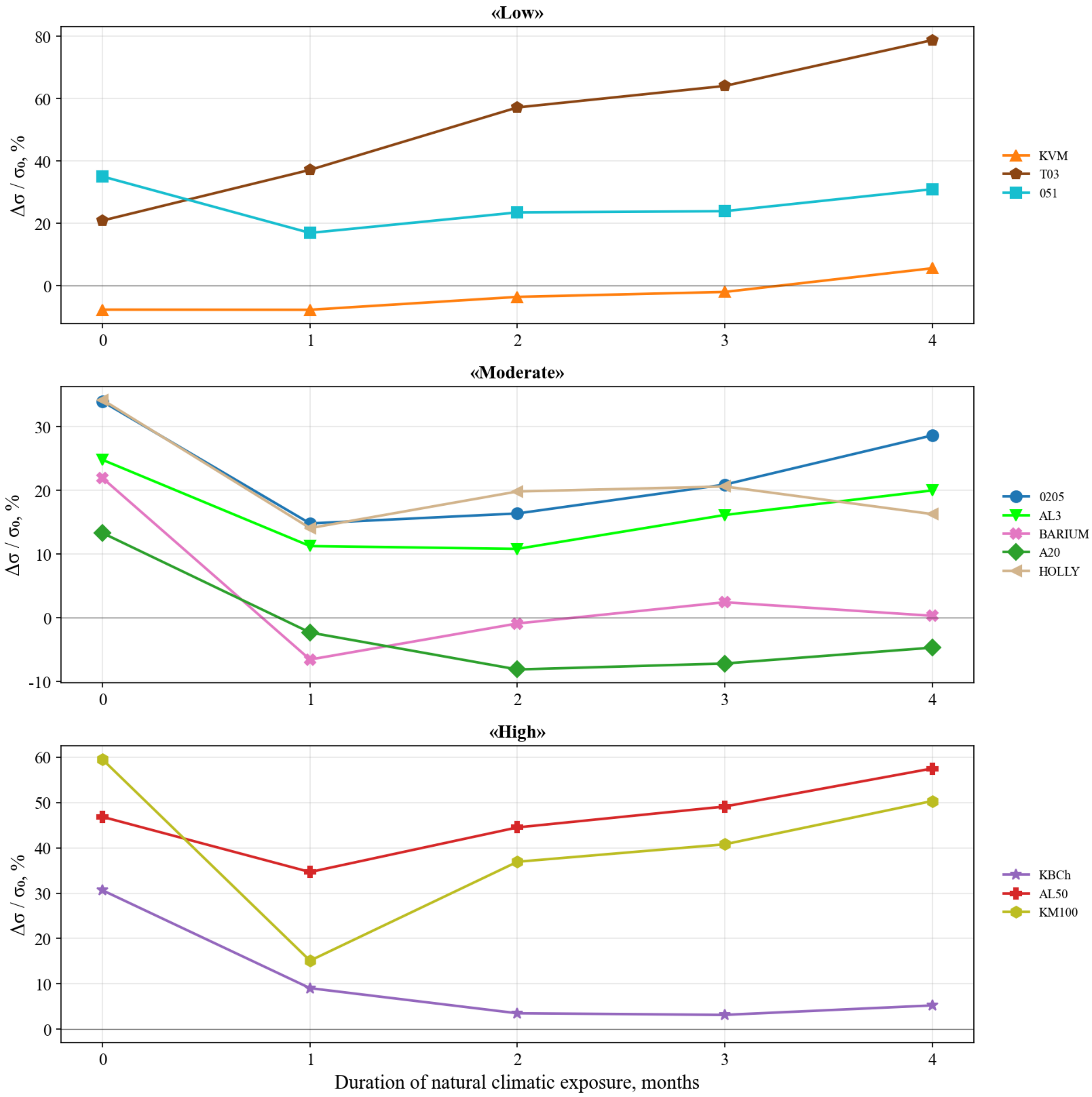

Fig. 9. Variation of the relative gain $\Delta\sigma$ of the specimens of the studied compositions in compression, calculated using the individual reference values for each measurement point, as a function of the duration of natural climatic aging.

Fig. 10 presents the dynamics of the change of the mean value of the yield strength under compression for the compositions of three conditional levels of the reinforcing effect, combined with the reference level of the unfilled 45M composition for all tested points. According to the presented data, in compression most filled composites retain the advantage over the unfilled matrix in the absolute strength at all time points.

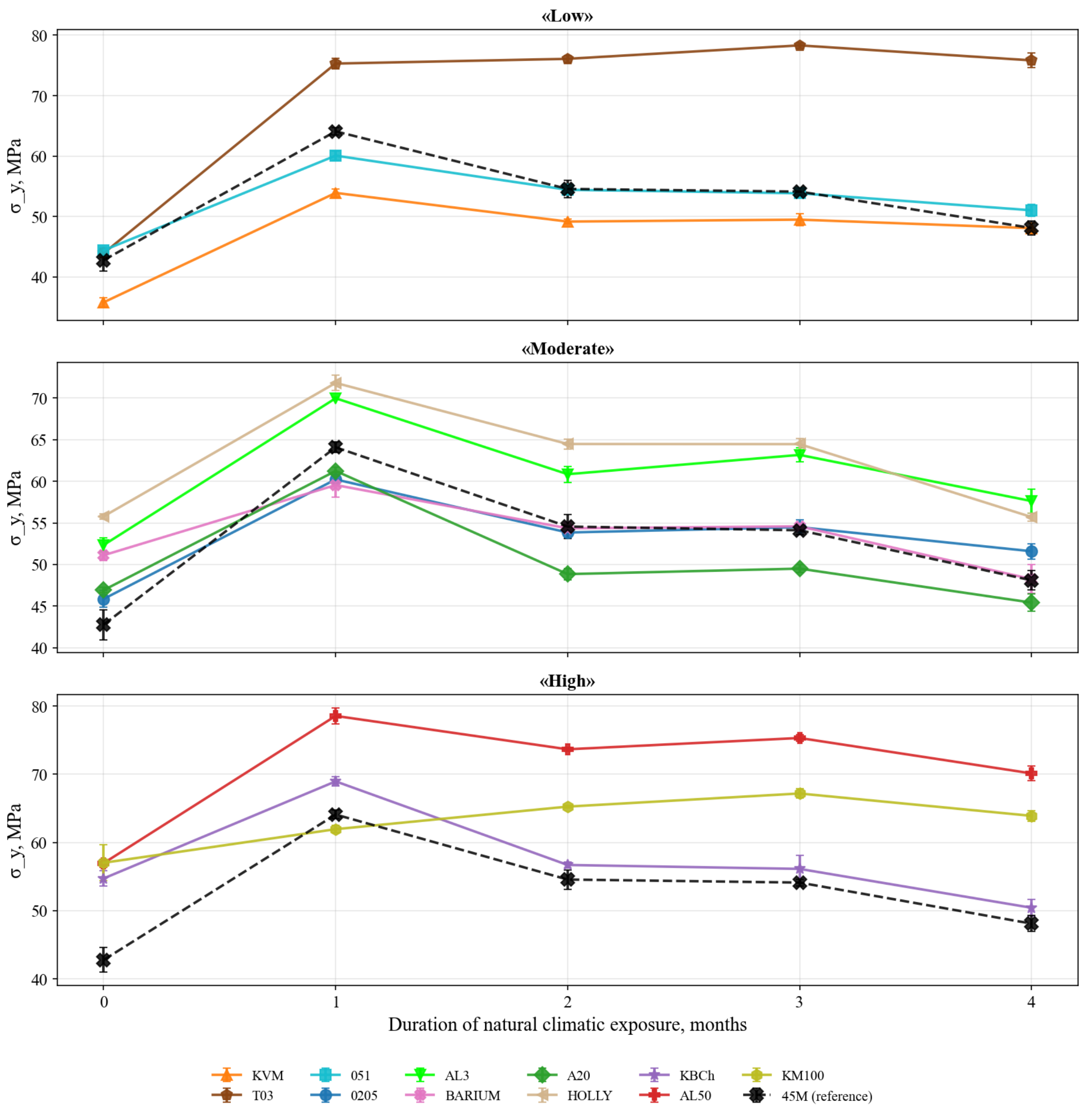

Fig. 10. Variation of the absolute values of the compression strength of the specimens of the studied compositions, grouped by the magnitude of the reinforcing effect $\Delta\sigma$.

The fundamental difference from the results obtained for bending loads (Fig. 6) consists in the smaller absolute spread between the groups (35–75 MPa vs. 30–95 MPa) – compressive loads lead to a levelling of the filler's contribution to the change of properties, reducing the expressiveness of the individual differences between the compositions. This circumstance indicates the lower informativeness of compression as a destructive method for monitoring the climatic degradation of polymer composites. As a consequence, bending and compression should be considered as two complementary target features of two models for predicting the mechanical properties of polymer composites. They reflect qualitatively different aspects of composite degradation – bending is more sensitive to the state of the surface and the phase boundary and provides greater differentiation between compositions, while compression is more sensitive to the bulk state of the material and demonstrates greater reproducibility between specimens. For practical applications related to predicting the residual service life of polymer composites in the process of natural operation, bending is characterised by greater relevance, which justifies the priority direction of work in this area. Nevertheless, both models retain independent value and are not reducible one to the other.

4. CONCLUSIONS

The experimental data obtained within the framework of the conducted research on the strength characteristics of epoxy polymer composites with mineral fillers under natural climatic aging allow the following conclusions to be formulated regarding the possibility of their use for training machine learning prediction models:

1. Based on the analysis of the two loading regimes, the relative indicator Δσ is proposed for use as the target feature of the models, representing the difference between the strength value (bending strength for bending; yield strength for compression) of the filled polymer material, corrected by the stresses (bending and compression, respectively) of the unfilled composition at the same level of relative strains. This approach automatically excludes from the target variable the components common to the unfilled 45M polymer and the filled composite associated with the post-curing effect and changes in the mechanical strength of the polymer matrix itself, while retaining as the main predicted effects the contribution of the filler to the change of properties and the state of the «polymer – filler» interface;

2. The difference in the choice of the reference indicator for calculating Δσ depending on the type of applied load is due to the fundamental difference between the σ–ε curves of the unfilled 45M polymer and those of the filled composites under bending and compression, respectively. Thus, if the introduction of a filler combined with bending loads in all cases without exception leads to an unambiguous transition from a viscous-fluid to a brittle failure mode described by a single point σ_y, then for compressive loads σ_{max} is, as a rule, located in the vicinity of extremely high relative strains (50 % and more), corresponding to the densification regime of the failed phase, which physically does not correspond to the real strength response of the studied materials. As a consequence, for the results in compression the yield strength σ_y was chosen as the indicator, representing the first local maximum on the σ–ε curve and available for unambiguous localisation and quantitative determination for all studied compositions;

3. The reference level σ_0, relative to which the indicators of the target feature Δσ for compression and bending are calculated, corresponds to the stress value obtained on the smoothed average σ–ε curve of the unfilled 45M composition at the point of relative strains ε_{ref}, calculated individually for each filled composition (for σ_{max} in bending and σ_y in compression). For each measurement point (reference state, 1–4 months of climatic aging), an individual reference σ–ε curve of the unfilled 45M composition is calculated, which provides reliable separation of the component of the current state of the polymer matrix that changes under the action of climatic aging;

4. Along with the proposed target feature of the model, it is advisable to include in the input feature space information about the type of filler (categorical), particle shape (categorical), mass fraction of the filler, characteristic particle size, specific surface area, and the relative strain at maximum load in the reference state (all – numerical);

5. Taking into account the relatively small volume of training samples available when using destructive monitoring methods, it is advisable for the prediction task to use gradient boosting algorithms and regularised linear models. This fact also constitutes a fundamental condition for the construction of accurate models, including careful feature engineering, control of overfitting, and regularisation;

6. The bending and compression indicators are considered as two independent target features, which is confirmed by the virtually zero correlation between them based on the obtained data. At the

same time, bending demonstrates substantially greater differentiation between compositions in terms of the reinforcing effect of filler introduction and more pronounced changes during natural climatic aging in comparison with compression. This is likely due to the difference in the orientation of the specimens during testing (face down for bending and face up for compression) and the natural difference in sensitivity to the accumulated surface degradation. As a consequence, from a practical viewpoint, the bending test results are of the greatest interest.

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