Evaluation of components influence of fillers in building materials on their physical characteristics by means of computer data analysis

A A Garashchenko

1 Irkutsk National Research Technical University, 83, Lermontov street, 664074 Irkutsk, Russia
E-mail: lamer_as@mail.ru

Abstract. The article presents an analysis of the dependence of the strength characteristics of new polymer-mineral composite building materials on the percentage of mineral filler components. The influence of the main components that are not included in the noncrystalline phase of the samples under study on the physical and mechanical properties of the materials under study was evaluated. The results showed that the use of substances with a high content of crystals with perfect splitting without crystals with imperfect splitting as fillers for a polymer composite could contribute to the production of building materials with high strength characteristics. These results can be used to assess the joint influence of components on both the physical characteristics already considered and others.

1. Introduction

Currently, research is actively conducted in order to find new fillers for the development of new building materials. In addition to developing technologies for the use of various biological structures (bacteria, fungi, algae, and others) as the basis for building material, investigations are underway to use other atypical mineral or organic fillers. One of the varieties of such research is the development of building materials that contain various industrial wastes as a filler. These studies make it possible to find a way to reuse industrial waste, which makes it possible in the future to reduce the total amount of waste and create new materials with special properties. It can be said that the creation of such building materials takes place under the auspices of creating eco-friendly household items in general.

There are projects to create eco-friendly household things that are familiar to us such as edible plastic bags, benches from old mobile phones, tetrapack ballpoint pens, plastic clothes and shoes and other examples. Similarly, there are projects to create building materials from old newspapers (NewspaperWood), animal blood (Blood Bricks), glass bottles, wine corks and others. One of the new fillers for construction materials considered in this article are wood dust, fly ash from the operation of Central Heating and Power Plants (CHPP), micromarble, vermiculite, microspheres, nanoparticles and others. Different wastes have a different composition of elements. These elements in different percentages and combinations with other components in a certain way affect the physical properties of the building material. Theoretically, this may allow one to obtain special construction materials, the physical properties of which are aimed at using in unusual conditions or instead of the usual materials with the elimination of their shortcomings.

This article presents a statistical study of the effect of the percentage of components on the strength
characteristics of new polymeric building materials developed over the past 5 years.

2. Materials and methods

For the study we used samples of new polymer-mineral composite materials, obtained over the past 5 years by extrusion method and conventionally called Vinisol (as a filler - fly ash), Vermiplast (as filler - vermiculite), Microplast (as a filler - ash microspheres), Marmaplast (as a filler, micromarble), nanoplast (with the addition of nanoparticles to fly ash). These materials contain mineral wastes of different types that seem promising from the point of view of the possibility of their use as fillers for the production of polymer composite materials. Mineral wastes from CHPP of the Irkutsk Region were mainly used.

To establish the quantitative characteristics of the phase (mineral) composition of the samples of the new building products, as well as the initial various fillers, X-ray phase analysis was performed. Powder X-ray diffraction data were obtained using a D8 ADVANCE Bruker diffractometer equipped with a scintillation detector and a Gbel mirror with step-by-step shooting in the 2θ diffraction angle range from 3 to 70 degrees using a CuKα radiation source. The experimental conditions were as follows (Table 1): 40 kV, 40 mA, exposure time - 1 s, step size - 0.02 ° 2θ. Data processing was performed using the software package DIFFRACplus. Samples were identified using the PDF-2 Powder Diffraction Database (ICDD, 2007) and indicated using EVA software (Bruker, 2007). In TOPAS 4 (Bruker, 2008), the relative percentage of phases was determined using the full-profile analysis using the Rietveld method. In a quantitative phase analysis using the Rietveld method, the contribution of the intensities of reflections of individual mineral gratings is estimated, depending on the variation of their profile and structural parameters. The amount of phase content is reduced to 100%.

Table 1 shows the numbers of the reference cards of the PDF-2 database [Release 2007], the names of the minerals used for the quantitative analysis, their chemical formulas, lattice parameters, space group and the strongest - identification - reflexes by which the phase was determined.

| Number  | Title  | Chemical formula | Symmetry, space group | E-cell options | Identification reflexes, d/n (hkl) |
|---------|--------|------------------|-----------------------|----------------|-----------------------------------|
| 01-070-3755 | Quartz | SiO₂            | Hexagonal P31           | a = 4.9158     | 3.345 (011)                       |
| 01-070-1469 | Fluorite | CaF₂           | Cubic Fm-3m            | a = 5.4502     | 3.147 (111), 1.927 (220)          |
| 00-036-0426 | Dolomite | CaMg(CO₃)₂      | Trigonal R₃            | a = 4.8092     | 2.888 (104)                       |
| 00-047-1743 | Calcite | CaCO₃          | Trigonal R₃c           | a = 4.9896     | 3.036 (104), 1.875 (11-6)         |

X-ray diffraction analysis was performed using the initial samples provided in the form of batten, after which powder samples were prepared from them, for which a repeated diffractogram was obtained. Samples in powder form were removed with a full filling of the standard cuvette (weighing 1-1.5 g). The total time taken to shoot a single diffractogram was about 70 minutes.

Table 2 presents the percentage of basic oxides per 1 gram of the studied materials. The remaining fraction is represented as an amorphous phase and oxides, which are specific to each of the materials presented for the study, therefore, they cannot be considered as factors affecting the physical and mechanical characteristics of the materials with sufficient confidence.
Table 2. A percentage of oxides in 1 gram of the studied material.

|          | Calcite (CaCO$_3$), % | Dolomite (CaMg(CO$_3$)$_2$), % | Fluorite (CaF$_2$), % | Quartz (SiO$_2$), % |
|----------|------------------------|-------------------------------|-----------------------|---------------------|
| Vinizol  | 2                      | 2                             | 2                     | 5                   |
| Vermiplast | 2                      | 7                             | 0                     | 3                   |
| Microplast | 1                      | 0                             | 1                     | 8                   |
| Marmaplast | 32                     | 5                             | 1                     | 0                   |
| Nanoplast | 18                     | 7                             | 1                     | 7                   |

The determination of the basic physical and mechanical parameters was performed in accordance with the State Standard of the Russian Federation (GOST) in the research center "Wood-Polymer Composites", Moscow.

Characterization of mineral-polymer compositions was carried out according to the following State Standards:

- bending strength GOST 4648
- modulus of flexibility GOST 9550
- bending strength of the profile board GOST 4648
- bearing capacity of distributed load per 1 m$^2$ of flooring GOST 4648
- rupture resistance GOST 11262
- Charpy impact strength GOST 4647.

One of the fundamental consumer properties, which largely determine the scope of application of building materials, is strength in its various manifestations.

Frequently used characteristics are ultimate tensile strength, compression and bending. They reflect the magnitude of the load applied to the material sample with which it is destroyed, depending on the cross-sectional area of the sample. Samples were prepared according to GOST 11262-80 and GOST 4651-2014.

Table 3 presents the results of the strength tests.

Table 3. Results of the strength tests.

|          | Bending strength, MPa | Modulus of flexibility, MPa | Rupture resistance, MPa | Charpy impact strength, kJ/m$^2$ | Bending strength of patterned lumber, N | Bearing capacity of distributed load per 1 m$^2$ of flooring (with the distance of 400 mm between the supports), kg |
|----------|------------------------|-----------------------------|-------------------------|-----------------------------------|----------------------------------------|---------------------------------------------------------------------|
| Vinizol  | 49.5                   | 5719                        | 21.8                    | 7.61                              | 4305                                   | 14795                                                               |
| Vermiplast | 54                     | 5836                        | 23.5                    | 14                                | 4430                                   | 15225                                                               |
| Microplast | 54.9                   | 3213                        | 25.6                    | 13.4                              | 3834                                   | 13176                                                               |
| Marmaplast | 29.9                   | 2406                        | 13.6                    | 5.62                              | 2567                                   | 8822                                                                |
| Nanoplast | 50.9                   | 5137                        | 21.1                    | 10.1                              | 4447                                   | 15283                                                               |

The data obtained from Table 2 and Table 3 were statistically processed. Statistical data processing was performed by means of Python 3.5.0 using NumPy 1.15.4.

3. Results and discussion
For each pair “oxide-characteristic” the linear Pearson correlation coefficient was calculated. The results of the calculations are presented in Table 4.

**Table 4. The linear Pearson correlation coefficients of the strength characteristics**

|                | Bending strength, MPa | Modulus of flexibility, MPa | Rupture resistance, MPa | Charpy impact strength, kJ/m² | Bending strength of patterned lumber, N | Bearing capacity of distributed load per 1 m² of flooring (with the distance of 400 mm between the supports), kg |
|----------------|-----------------------|-----------------------------|-------------------------|-------------------------------|----------------------------------------|------------------------------------------------------------------|
| Calcite        | 0.447                 | 0.633                       | 0.315                   | 0.602                         | 0.579                                  | 0.579                                                            |
| Dolomite       | 0.821                 | 0.276                       | 0.785                   | 0.813                         | 0.655                                  | 0.655                                                            |
| Fluorite       | -0.186                | 0.569                       | -0.295                  | -0.566                        | 0.21                                   | 0.21                                                             |
| Quartz         | -0.703                | -0.459                      | -0.744                  | -0.849                        | -0.529                                 | -0.529                                                           |

As can be seen from Table 3, the large presence of quartz in the composition has a pronounced negative impact on all the above physical and mechanical characteristics. Of all the oxides studied, dolomite has the greatest positive effect on these characteristics. This phenomenon is associated with different splitting of quartz and dolomite. Quartz has an imperfect cleavage, so it has high hardness and high brittleness. Thus, the presence of quartz generally reduces the strength of the material. On the other hand, dolomite, which has perfect cleavage, has a softer, more viscous structure, which makes it less brittle. Thus, dolomite, as a rule, increases the strength of the material, with the exception of the flexural modulus. Calcite and fluorite have a more pronounced positive effect on this characteristic. However, fluorite does not have a completely positive effect on the physical characteristics of the considered building materials, unlike calcite, the presence of which, albeit to a slightly lesser extent than dolomite, also has a positive effect on the resulting characteristics. Perhaps this is due to the fact that, despite the perfect cleavage of both elements, fluorite has a slightly more solid structure than calcite. It is also possible that the combination of calcite and dolomite affects mostly the physical characteristics of building materials. It makes sense to study the effect of components in a pair on the strength characteristics of building materials.

### 4. Conclusion

After research, we can conclude that the use of substances with a high content of crystals with perfect splitting as fillers for the polymer composite can contribute to the production of building materials with high strength characteristics. At the same time, minerals with the lowest content of crystals with imperfect cleavage should be used, since they, in general, can have a negative effect on the target characteristics. It may be necessary to remove these crystals at all.

Additional studies with a large number of experimental samples may reveal the dependence of the strength characteristics of combinations of various substances in the composition of materials. For a better effect, it will be possible to test this hypothesis both on the basis of the components already mentioned in the article, and on the example of other possible fillers for polymer-mineral composites.

Research in the development of environmentally friendly items and, in particular, building materials is aimed at creating new ways of possible waste disposal and reuse of recyclables. In the future, this approach will allow us not to suffer from the lack of our usual resources, since many of the things we have created can be considered as new independent sources of missing resources. Thus, it is possible to postpone significantly the emergence of a resource crisis.
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