# Prediction of the modulus of elasticity of building materials based on wood-polymer composites.

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**Abstract**

Methods for predicting the elastic modulus of materials based on thin dispersions of one of the polymers in the polymer matrix of another polymer are considered. The options are analyzed: dispersion of a solid amorphous polymer of a certain chemical structure in a solid amorphous polymer matrix of a different chemical structure; the dispersion of mineral filler particles in a composite matrix based on a mixture of organic polymers. The preparation of wood-polymer composites increases the elastic modulus from 2400 to 4660 MPa under tensile conditions. The introduction of a mineral filler in the form of CaCO3 leads to an increase in the E modulus to 3230 MPA with a CaCO3 content relative to the wood filler of 42%. The prediction of the elastic modulus for composites containing moso bamboo as a wood filler shows that with this content of wood filler, the modulus of elasticity can increase to 4400 MPa.

**Key words:** polyvinyl chloride, polymer compatibility, modulus of elasticity, van der Waals volume, wood-polymer composites.

**Introduction**

To date, the mechanical properties of a large number of polymer mixtures have been studied, but only a few studies are devoted to calculation methods of forecasting. Briefly consider these works. For mixtures of polystyrene and ABS plastic, it was found that their mechanical properties are better than similar properties of constituent components [1]. The authors attribute this to the good compatibility of these polymers. In [2], various calculation methods for estimating the dependences of the modulus of elasticity on the composition of mixtures were considered. These dependencies are often extreme and have maxims, i.e. the elastic moduli of mixtures can exceed the average values for different compositions.

The morphology and properties of mixtures of polystyrene with a copolymer of styrene and acrylonitrile were studied. The measured elastic moduli of the mixtures were compared with the calculated values that were described using the Doi theory [3]. Found that the main role is played by an increase in particle size associated with a change in interfacial tension and viscosity of the mixtures. The effect of interfacial tension in incompatible polymer mixtures was studied in a number of works [4–8].

Despite the large number of papers devoted to the structure and mechanical properties of mixtures, the issues analyzed in this paper do not always find an adequate consideration. First of all, this refers to the possibility of predicting the compatibility of polymers based on their chemical structure and phase state, assessing the elastic modulus of the mixture taking into account the phase and physical state of the mixed polymers (dispersion of a solid polymer in an elastomer, dispersion of two solid, glassy or crystalline polymers). In this case, chemical interaction between microphases is possible. All this affects the elastic modulus of materials based on polymer blends. This article discusses the dispersion of solid polymer 1 in solid polymer 2.

To analyze the modulus of elasticity $E$ of the mixture, we use the formula obtained in [9] and transform it:

$$E = \frac{\alpha_{m,p1}\left(\sum_i \Delta V_i\right)_{p,1} + \alpha_{m,p2}\left(\sum_i \Delta V_i\right)_{p,2} + \cdots + \alpha_{m,pn}\left(\sum_i \Delta V_i\right)_{p,n}}{\dfrac{\alpha_{m,p1}\left(\sum_i \Delta V_i\right)_{p,1}}{E_1} + \dfrac{\alpha_{m,p2}\left(\sum_i \Delta V_i\right)_{p,2}}{E_2} + \cdots + \dfrac{\alpha_{m,pn}\left(\sum_i \Delta V_i\right)_{p,n}}{E_n}} \tag{1}$$

In the formula (1) $\left(\sum_i \Delta V_i\right)_{p1}$, $\left(\sum_i \Delta V_i\right)_{p,2}$, $\left(\sum_i \Delta V_i\right)_{p,n}$ are the van der Waals volumes of the repeating units (or repeating network fragments) of polymers 1, 2, and $n$, respectively; $\alpha_{m,1}$, $\alpha_{m,2}$ and $\alpha_{m,n}$, $n$ are the molar fractions of polymers 1, 2 and $n$, respectively; $E_1$, $E_2$ and $E_n$ are the elastic moduli of polymers 1, 2, and $n$, respectively.

In a more compact form, equation (1) is written as

$$E = \frac{\sum_{k=1}^{k=n} \alpha_k \left(\sum_i \Delta V_i\right)_k}{\sum_{k=1}^{k=n} \alpha_k \dfrac{\left(\sum_i \Delta V_i\right)_k}{E_k}} \tag{2}$$

where $\alpha_k$ is the mole fraction of the $k$-th component, $\left(\sum_i \Delta V_i\right)_k$ is the van der Waals volume of the $k$-th component, $E_k$ is the elastic modulus of the $k$-th component.

Given that for a two-component system $\alpha_{m,1} + \alpha_{m,2} = 1$, equation (1) is written as

$$E=\frac{1+\alpha_{m,2}\left[\frac{\left(\sum_i \Delta V_i\right)_2}{\left(\sum_i \Delta V_i\right)_1}-1\right]}{\frac{1}{E_1}+\alpha_{m,2}\left[\frac{\left(\sum_i \Delta V_i\right)_2}{\left(\sum_i \Delta V_i\right)_1 E_2}-\frac{1}{E_1}\right]} \qquad (3)$$

In equation (3) $\left(\sum_i \Delta V_i\right)_1$ and $\left(\sum_i \Delta V_i\right)_2$ are the van der Waals volumes of the repeating units (or repeating network fragments) of polymers 1 and 2, respectively; $\alpha_{m,1}$ and $\alpha_{m,2}$ are the molar fractions of polymers 1 and 2, respectively; $E_1$ and $E_2$ are the elastic moduli of polymers 1 and 2, respectively.

In order to obtain the dependence of the modulus of elasticity on the weight fraction of polymers $\alpha_w$, we use the relationship between the molar and weight fractions:

$$\alpha_{m,2}=\frac{1}{1+\frac{M_{p2}}{M_{p1}}\left(\frac{1}{\alpha_{w,2}}-1\right)} \qquad (4)$$

Then, the dependence of the modulus of elasticity on the weight fraction of the second polymer $\alpha_{w2}$ is written as

$$E=\frac{1+\frac{\left[\left(\sum_i \Delta V_i\right)_{p2}\Big/\left(\sum_i \Delta V_i\right)_{p1}-1\right]}{1+\frac{M_{p2}}{M_{p1}}\left(\frac{1}{\alpha_{w2}}-1\right)}}{\frac{1}{E_1}+\frac{\left(\frac{\left(\sum_i \Delta V_i\right)_{p2}\Big/\left(\sum_i \Delta V_i\right)_{p1}}{E_2}-\frac{1}{E_1}\right)}{1+\frac{M_{p2}}{M_{p1}}\left(\frac{1}{\alpha_{w2}}-1\right)}} \qquad (5)$$

To obtain a significant increase in the elastic modulus of the mixture, it is necessary to analyze the dependence of the elastic modulus on the content of the natural polymer – wood. Wood is introduced into the technological mixture with PVC, as a result of which the elastic modulus increases significantly. To calculate the elastic modulus, it is necessary to know the composition of wood of different species and the physical parameters of PVC and wood components. These parameters are borrowed from literary sources [10-12] and are in tables 1 and 2.

**Table 1. The basic composition of wood**

| Wood | Cellulose | Lignin | Hemicellulose |
|---|---|---|---|
| Conifers | 42.5 % | 28.5 % | 22.5 % |
| Moso bamboo | 44.6 % | 20.3 % | 23.6 % |

**Table 2. Physical parameters of the main components of coniferous wood**

| Wood components | Molecular weight of the repeating unit | Van der-Waals volume, Å$^3$ | Density, g/cm$^3$ |
|---|---|---|---|
| Cellulose | 162 | 102.6 | 1.54 |
| Lignin | 340 | 302 | 1.23 |
| Hemicelluloses | 292 | 203 | 1.40 |

The molecular weight of wood, which is the second polymer introduced into the mixture with PVC, was calculated by the formula

$$M_2 = \alpha_C \cdot M_C + \alpha_L \cdot M_L + \alpha_{HC} \cdot M_{HC} \qquad (6)$$

where $\alpha_C$, $\alpha_L$ and $\alpha_{HC}$ are the proportions of cellulose, lignin and hemicelluloses, respectively, $M_C$, $M_L$ and $M_{HC}$ are the molecular weights of cellulose, lignin and hemicelluloses, respectively.

The molecular weights of lignins and hemicelluloses are taken into account as average values. For example, for hemicelluloses, the average value was calculated on the basis of molecular weights for 16 hemicelluloses of various chemical structures. These data are given in the monograph [10].

In a similar way, the van der Waals volumes of wood were calculated:

$$\left(\sum_i \Delta V_i\right)_2 = \alpha_C \cdot \left(\sum_i \Delta V_i\right)_C + \alpha_L \cdot \left(\sum_i \Delta V_i\right)_L + \alpha_{HC} \cdot \left(\sum_i \Delta V_i\right)_{HC} \qquad (7)$$

where $\left(\sum_i \Delta V_i\right)_C$, $\left(\sum_i \Delta V_i\right)_L$ and $\left(\sum_i \Delta V_i\right)_{HC}$ are the van der Waals volumes of cellulose, lignin and hemicelluloses, respectively.

Using the values of all parameters in tables 1 and 2, using the equation (5), we obtained the dependences of the elastic modulus on the weight fraction of coniferous wood and moso bamboo, shown in Figure 1.

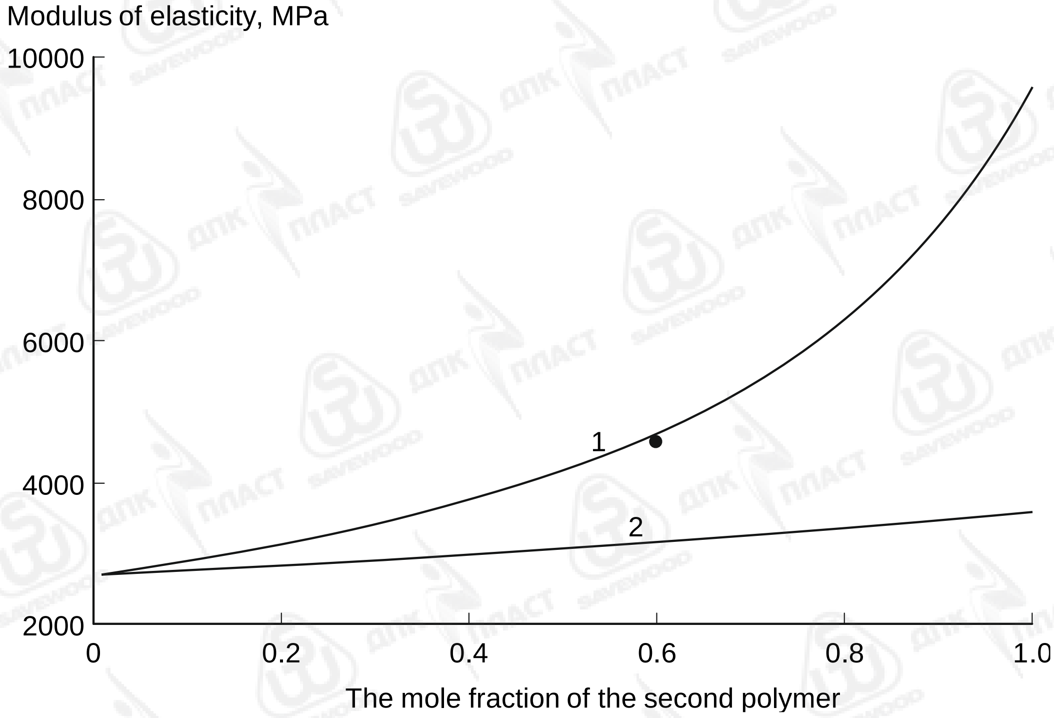


Fig. 1. The dependences of the elastic modulus on the weight fraction of the second polymer. 1 - coniferous wood, 2 - moso bamboo wood.

This figure shows the elastic moduli measured by tensile composites of PVC with wood. The elastic modulus of a composite of coniferous wood increases significantly with increasing concentration of wood. When the ratio of PVC to wood is 40:60, which is used in the manufacture of composites at the Russian company Savewood, the tensile modulus is increased from 2400 MPa to 4660 MPa. This is reflected by a point on curve 1 in the graph. As can be seen from the graph, the experimentally measured elastic modulus coincides well with the calculated modulus. When moso bamboo is introduced into PVC, the tensile modulus also increases, but not so much compared to the modulus of elasticity when softwood is introduced. This conclusion needs experimental confirmation.

Now we analyze the dependence of the elastic modulus of composites in which part of the wood flour is replaced with a mineral filler $CaCO_3$. Equation (5) allows you to calculate the dependence of the elastic modulus on the weight fraction of the filler. To do this, you first need to determine the density $\rho_p$ of the polymer binder. The calculation is carried out according to the formula

$$\rho_p = (\alpha_C \cdot \rho_C + \alpha_L \cdot \rho_L + \alpha_{HC} \cdot \rho_{HC}) \cdot 0.6 + \rho_{PVC} \cdot 0.4 \quad (8)$$

where $\alpha_C$, $\alpha_L$ and $\alpha_{HC}$ are the proportions of cellulose, lignin and hemicelluloses, respectively, $\rho_C$, $\rho_L$, $\rho_{HC}$ and $\rho_{PVC}$ are the densities of cellulose, lignin, hemicellulose and polyvinyl chloride, respectively.

The densities ρ and weight fractions of the wood components are given in tables 1 and 2. The binder containing 40% PVC and 60% wood flour was used. Elastic moduli were determined from stress-strain curves at compression measured for all samples containing different amounts of $CaCO_3$. Parallel measurements were carried out for three samples of each series. The measurements were carried out on a device for micromechanical testing of the Dubov-Regel design, which we modified to convert the readings of a photoelectro-optical dynamometer into an electrical signal which are recorded using a galvanometer. All data is automatically recorded on the computer, including the results of measurements and calculations. We used samples 4×4×6 mm in size with plane-parallel faces. The compression rate was 0.187 mm/min. As an example, stress-strain curves at compression are shown in Figure (2) for a composite containing 40% $CaCO_3$ with respect to wood.

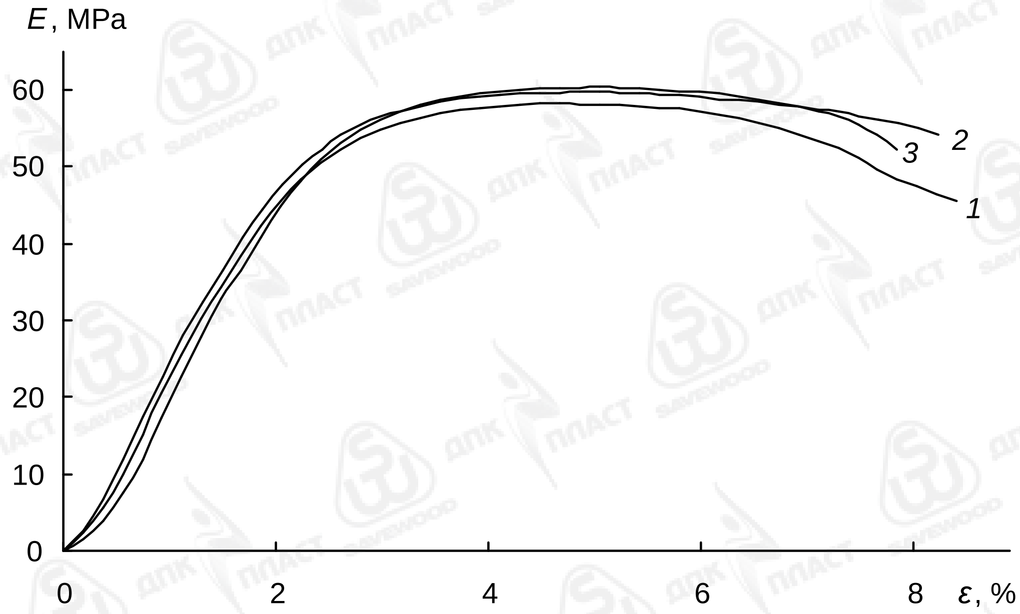


Fig. 2. Stress-strain curves at compression of the samples of composites containing a polymer binder and the mineral filler. The $CaCO_3$ content is 40% with respect to wood.

The values of the modulus of elasticity are shown in table 3.

**Table 3. Moduli of elasticity of samples of composites under compression**

| Sample | Share of $CaCO_3$, % | The average modulus of elasticity, MPa |
|---|---|---|
| *а* | 0 | 1930 |
| *б* | 30 | 2660 |
| *в* | 40 | 2900 |
| *г* | 60 | 3230 |
| $CaCO_3$ | 100 | 6500 |

The modulus of elasticity was predicted for a 2-component system. The first component is a wood-polymer composite containing PVC and wood flour obtained from conifers or moso bamboo. The second component is $CaCO_3$. Since this component is not organic, its van der Waals volume cannot be calculated using the Cascade computer program. Therefore, the effective van der Waals volume can be calculated according to equation (5) using the experimental value of the $E_2$ for the composite containing the largest amount of $CaCO_3$ equal to 70% with respect to wood flour. Since the concentration of wood flour in the composite is 60%, the concentration of $CaCO_3$ is 70×0.6 = 42%. The equation to be used follows from formula (5):

$$E = E_{p1}\frac{\left(\sum_i \Delta V_i\right)_{p1}\cdot\frac{M_{CaCO}}{M_{p1}}\left(\frac{1}{\alpha_{wCaCO_3}}-1\right)-\left(\sum_i \Delta V_i\right)_{CaCO_3}}{\left(\sum_i \Delta V_i\right)_{p1}\cdot\frac{M_{CaCO}}{M_{p1}}\left(\frac{1}{\alpha_{wCaCO_3}}-1\right)+\frac{E_1}{E_2}\left(\sum_i \Delta V_i\right)_{CaCO_3}-\left(\sum_i \Delta V_i\right)_{p1}} \quad (9)$$

Index $p1$ means that all calculated values refer to a polymer binder consisting of PVC and wood. The molecular weights of the wood components and their weight fractions are presented in Tables 1 and 2, and the elastic modulus $E_1$ for the wood-polymer composite that does not contain a mineral filler is 1930 MPa. The average modulus of elasticity $E_2$ for $CaCO_3$ is equal to 6500 MPa. The experimental value of the elastic modulus of the composite under consideration is $E$ = 3230 MPa. Substitution of all parameter values into equation (9) leads to the value $\left(\sum_i \Delta V_i\right)_{CaCO_3}$ = 140 Å3. Using this value, we can calculate the elastic modulus according to equation (5) for all concentrations of the mineral filler and compare with experimental data. As a result, we obtain the dependence of the elastic modulus on the concentration of $CaCO_3$, shown in Fig. 3.

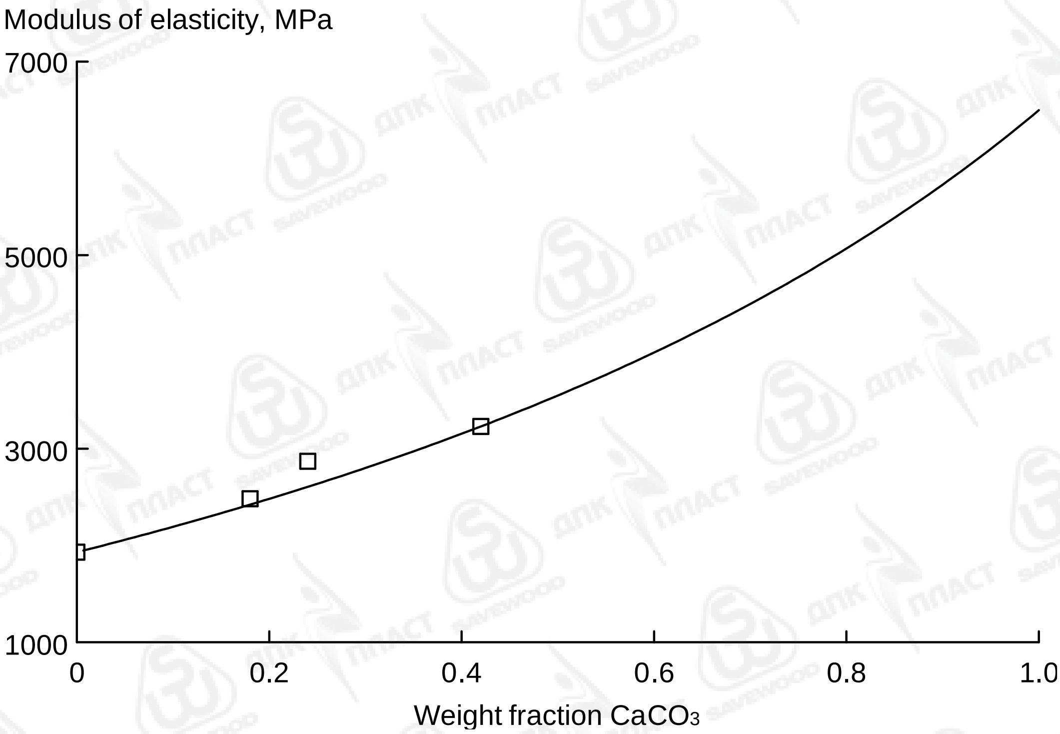


Fig. 3. The dependence of the elastic modulus on the weight fraction of $CaCO_3$ with respect to wood filler. The curve is calculated, the points are experimental

From table 3 and figure 3 it is seen that the modulus of elasticity in compression is increased with increasing concentration of the mineral filler. At the same time, we can conclude that the experimental values of the elastic moduli coincide with the calculated values.

We perform the same calculations for composites containing the mixture of PVC and moso bamboo as a matrix polymer [11]. The calculations were performed according to formulas (6), (7) and (8). The calculation results are as follows. The molecular weight of the mixture is $M_{p1}$ =

210, van der Waals volume $\left(\sum_i \Delta V_i\right)_{p1}$ = 155 Å$^3$. Substitution of these parameters into equation (9) leads to the dependence of the elastic modulus on the weight fraction of $CaCO_3$ shown in Figure 4.

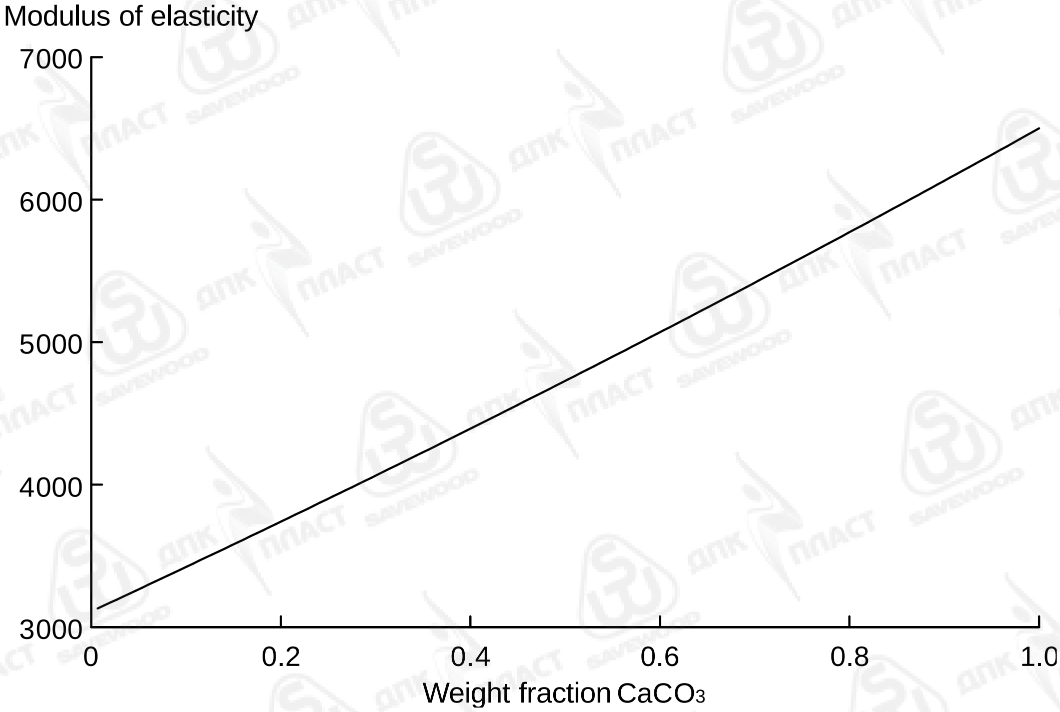


Fig. 4. The dependence of the elastic modulus on the weight fraction of $CaCO_3$ with respect to the wood filler (moso bamboo).

A comparison of Figures 3 and 4 shows that the elastic modulus for any moso bamboo content is higher than the elastic modulus of composites containing coniferous wood flour. However, in the analysis of these dependences for composites containing softwood flour, the experimental values of the elastic modulus $E_{p1}$ were used, and for composites containing moso bamboo, only the calculated value $E_{p1}$ = 3110 MPa was used. In the future, experiments should be performed to measure stress-strain curves at compression for such composites and compare the results of experiments and calculations.

As a result of the work carried out, we can draw the following conclusion about predicting the elastic modulus of PVC-based composites. The introduction of wood filler into PVC increases the elastic modulus from 2400 to 4660 MPa under tensile conditions. The introduction of a mineral filler in the form of $CaCO_3$ leads to an increase in the $E$ modulus to 3230 MPa with a $CaCO_3$ content relative to the wood filler of 42%. The prediction of the elastic modulus for composites containing moso bamboo as the wood filler shows that with this content of wood filler, the modulus of elasticity can increase to 4400 MPa.

In general, the possibility of calculating the elastic moduli of materials based on polymer mixtures was demonstrated by the example of dispersion of solid polymer 1 in solid polymer 2, as well as by the example of dispersion of the mineral filler in a solid polymer matrix. The dependences of the elastic moduli on the molar and volume fractions possess different shapes associated with the van der Waals volume of the components, the molecular mass of the repeating units, and the density of the components. It was found that the elastic modulus is increased with increasing concentration of polymers in a mixture with PVC, which possess a high glass transition temperature. The addition of the mineral filler to a mixture of PVC and wood contributes to an increase in the modulus of elasticity.

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