



Mathematical Model of the Mechanical Activation Process of the Initial Components of Metal Matrix Nanocomposites

Vadim KOVTUN¹, Vladimir PASOVETS^{1,2}, Yordan MIRCHEV³

¹ University of Civil Protection of the Ministry for Emergency Situations of the Republic of Belarus, Belarus,
Phone: +375173454086, Fax: +375173403557, e-mail: vadimkov@ya.ru

² State Research and Production Powder Metallurgy Association National Academy of Sciences of Belarus,
Minsk, Belarus, Phone: +375172928271, Fax: +375172100574, e-mail: pasovets_v@mail.ru

³ Institute of Mechanics of the Bulgarian Academy of Sciences, Sofia, Bulgaria;
e-mail: mirchev@imbm.bas.bg, nmtdd@abv.bg

Abstract

A mathematical model of the process of mechanical activation of the initial components of nanocomposites with a metal matrix has been developed. This model is based on the mathematical description of the processes of van der Waals interaction of carbon nanostructures, their separation and distribution at the mechanical activation. The mathematical model, taking into account the criteria for the effective separation of agglomerates of carbon nanostructures and distribution carbon nanostructures in the process of mixing nano- and micro-sized initial components of composite materials, makes it possible to determine the energy values of the van der Waals interaction of carbon nanostructures, the energy values supplied by the mixer-activator at given technological parameters of mechanical activation, and also to predict the optimal time of mechanical activation of a powder system of various masses, sufficient for the destruction of agglomerates of carbon nanostructures and their distribution in a powder metal matrix.

Keywords: powder, nanocomposite, mathematical model, carbon nanotube, agglomerate, mechanical activation, van der Waals interaction.

1. Introduction

Composite materials with a metal matrix filled of carbon nanostructures materials really promising for practical application in the mechanical engineering, automotive and aviation industries. Powders of both pure metals and their alloys are used as matrices of these materials. Carbon nanotubes (CNTs) are the most studied and used carbon nanostructured filler [1, 2].

The distribution of carbon nanostructures in a metal micro-sized matrix is a serious problem. Nanosized filler tends to form micro-sized agglomerates [3]. The process of distribution of a nano-sized filler in a metal matrix can be interpreted as the supply of mechanical energy to the initial components of the powder system for the separation of micro-sized agglomerates and fixing carbon nanostructures on the surface of micro-sized particles of a metal matrix. In this case, the counteracting factor that makes difficult of separation the nanosized components is the binding energy that keeps the nanoparticles in the agglomerate.

Thus, it is possible to establish criteria for the effective degradation of agglomerates and separation of CNTs in the process of mixing nano- and micro-sized initial components of composite materials. First, the applied energy must exceed the binding energy of CNT agglomerates. This will break up the micro-sized agglomerates of nanoparticles. Second, the amount of energy supplied should not exceed the energy required to destroy a single CNT. This will make it possible to preserve the structure and high physical and mechanical characteristics of individual CNTs. Therefore, the optimal method for separating agglomerates of a nanosized filler should provide a lower limit of the applied energy sufficient to break the bond of agglomerates and an upper limit of energy insufficient to destroy individual CNTs [4].

For the destruction of agglomerates of carbon nanostructures and distribution of carbon nanostructures in a metal matrix, it is reasonable to use mechanical activation methods. Supply additional energy to the powder system makes it possible to separate and distribute nanosized components in a metal micro-sized matrix. Replacing the mixing process with mechanical activation prevents the segregation of carbon nanostructures and their subsequent re-agglomeration. Thus, the purpose of the work was to develop a mathematical model of the process of mechanical activation of the initial components of nanocomposites with a metal matrix.

2. Mathematical model

The shape and geometric dimensions of CNTs differ. The forces of interaction between pairs of nanotubes can be estimated using theoretical models.

The van der Waals interaction of two CNTs was analysed using the Hamaker constant [5]. In this case, the interaction energy was determined by modeling each CNT as a mesoscale rod continuum [6]. It was experimentally shown in [7] that for the van der Waals attraction between the outer layer of a multilayer CNT and a metal surface in vacuum, the Hamaker constant is $A_H = 60 \times 10^{-20}$ J.

It can be assumed that this constant between the side walls of the CNT will differ slightly from the given value. Knowing the Hamaker constant, one can determine the energy of the van der Waals interaction between a pair of parallel CNTs. The solution of this problem is similar to the solution that describes the van der Waals interaction energy between two parallel mesoscopic cylinders of length l , diameter d_{CNT} , separated by a gap H [8]:

$$E_{//} \approx \frac{A_H}{24} \cdot l \cdot d_{CNT}^2 \cdot H^{-3} \text{ in case } H \geq H_c \quad (1)$$

where A_H is Hamaker's constant, $A_H = 60 \times 10^{-20}$ J; l is the CNT length, m; d_{CNT} is the CNT diameter, nm; H is the distance between interacting CNTs, m; H_c is the distance between the graphene layers of a multilayer CNT, $H_c = 3.4 \times 10^{-20}$ m.

The interaction energy of two CNTs can be modeled by two perpendicularly crossed rods of diameter d_{CNT} located at a distance H [8]:

$$E_+ \approx \frac{A_H}{12} \cdot \frac{d_{CNT}}{H} \text{ in case } H < d_{CNT} \quad (2)$$

Energy of van der Waals interaction of carbon nanosized filler in the sample:
- for parallel arrangement:

$$E_p = 0.5n_{CNT} \cdot E_{//} \quad (3)$$

where n_{CNT} is number of CNTs in the sample, pcs.

- for cross arrangement:

$$E_c = 0.5n_{CNT} \cdot E_+ \quad (4)$$

Total interaction energy:

$$E_o = E_p + E_c \quad (5)$$

The homogeneous distribution of CNTs in the metal matrix determines the properties of the composite and is a significant problem. Thus, the influence of the spatial arrangement of the carbon nanostructured filler on the value of the agglomeration energy has been shown.

Based on the analysis of the presented formulas, we can draw the following conclusions. The energy values of the van der Waals interaction in the case of a parallel arrangement of CNTs significantly exceed the energy values in the case of a crossed arrangement, which is explained by the significant length of the interaction. Increasing the distance between interacting CNTs significantly reduces the interaction energy [4].

However, deagglomerated CNTs tend to form new agglomerates. Therefore, they must be fixed on the surface of micro-sized particles of the copper matrix.

Let us calculate the energy required to fix CNTs on the surface of matrix particles. This energy will be the work that needs to be done to introduce CNTs into the copper matrix, subject to its local deformation.

The energy required for the introduction of CNTs into the copper surface:

$$E_{CNT-Cu} = n_{CNT} \cdot \sigma_{TCu} \cdot S_{CNT} \cdot \delta \quad (6)$$

where σ_{TCu} is the yield strength of the matrix metal, for copper $\sigma_{TCu} = 68.5$ MPa; S_{CNT} is the CNT projection area, m^2 ; δ is the penetration depth of CNTs, m.

$$S_{CNT} = l \cdot d_{CNT} \quad (7)$$

Also, in the process of mechanical activation, energy is spent on the deformation of the particles of the metal matrix. The amount of energy for deformation of matrix particles can be calculated as follows:

$$E_{Cu} = n_{Cu} \cdot \sigma_{TCu} \cdot S_{Cu} \cdot \delta_{Cu} \quad (8)$$

where S_{Cu} is the projection area of a copper particle, m^2 ; δ_{Cu} is the value of deformation of copper particles, μm ; n_{Cu} is the number of matrix particles in the sample, pcs.

$$S_{Cu} = \frac{\pi \cdot d_{Cu}^2}{4} \quad (9)$$

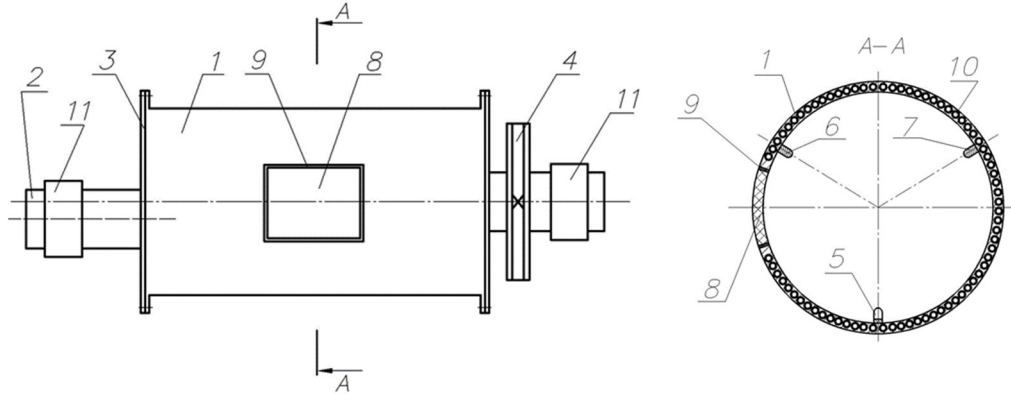
where d_{Cu} is the copper particle diameter, m.

The amount of energy supplied to the activated system per unit time [9]:

$$P = 0.5 \cdot K_a \cdot K_b^2 \cdot K_v \cdot m_b \cdot \left(\frac{\pi \cdot n}{30}\right)^3 \cdot R^2 \cdot N_b \quad (10)$$

where K_a is the coefficient depending on the elasticity of the impact; K_b is a constant that depends on the geometry of the working elements of the mixer-activator; K_v is a constant depending on the design features of the working chamber of the mixer-activator; m_b – mass of one active working body, kg; n – frequency of rotation of the working chamber, min^{-1} ; R is the radius of the circle of the working chamber of the mixer-activator, m; N_b – the number of active working bodies; t is the operating time of the mixer-activator, s.

The design of the mixer-activator is shown in Figure 1. This mixer-activator creates percussion effect, rolling, intensive mixing and activation of the surface of the initial components of the powder composite material under the action of vibration. As a result, a sufficiently uniform distribution of the nanosized filler in the metal micro-sized matrix is ensured [10].



1 – working chamber; 2 – axles; 3 – flanges; 4 – drive; 5–7 – ridges; 8 – cover;
9 – sealant; 10 – heating elements; 11 – contact bushings

Fig 1. Mixer-activator

Thus, the energy calculation of the process of preliminary mechanical activation of copper-CNT powder systems showed that the amount of energy supplied depends on the rotation frequency and dimensions of the working chamber of the mixer-activator, the diameter and material of the active working bodies. Comparing the required amount of energy with the amount of energy supplied when using a mixer-activator, it is possible to calculate the time of mechanical activation:

$$t(n) = \frac{0.5n_{CNT} \cdot \left(\frac{A_H}{24} \cdot l \cdot d_{CNT}^{\frac{1}{2}} \cdot H^{-\frac{3}{2}} + \frac{A_H}{12} \cdot \frac{d_{CNT}}{H} \right) +}{0.5 \cdot K_a \cdot K_b^2 \cdot K_v \cdot m_b \cdot \left(\frac{\pi \cdot n}{30} \right)^3 \cdot R^2 \cdot N_b} + \frac{n_{CNT} \cdot \sigma_{TCu} \cdot S_{CNT} \cdot \delta + n_{Cu} \cdot \sigma_{TCu} \cdot S_{Cu} \cdot \delta_{Cu}}{0.5 \cdot K_a \cdot K_b^2 \cdot K_v \cdot m_b \cdot \left(\frac{\pi \cdot n}{30} \right)^3 \cdot R^2 \cdot N_b} \quad (11)$$

$$m_b = \frac{4\pi \cdot r_b \cdot \rho_b}{3} \quad (12)$$

where r_b is the radius of the working body, m; ρ_b is the density of the material of the working body of the mixer-activator, kg/m³.

Border conditions:

$$\begin{aligned} H &\geq H_c \\ H &< d_{CNT} \\ \delta &\leq d_{CNT} \\ \delta_{Cu} &< d_{Cu} \\ n &\leq n_{cr} \end{aligned} \quad (13)$$

where n_{cr} – critical frequency of rotation of the working chamber, min⁻¹.

Thus, a mathematical model of the distribution of carbon nanostructures in a powder metal matrix has been developed. The model is based on the ongoing physical processes at the technological stage of activation. This mathematical model takes into account the shape, size and properties of the initial dispersed components of various structural levels, the rotation frequency and design features of the working chamber of the mixer-activator. The developed model makes it possible to establish the optimal time of mechanical activation of a powder system of various masses, which is sufficient for the destruction of agglomerates of carbon nanostructures and their distribution in a powder metal matrix.

The analysis of the developed mathematical model made it possible to draw the following conclusions. For a composite system based on a copper matrix filled with 0.07 wt. % of CNTs, the amount of mechanical energy supplied over a period of 55 to 60 minutes at a frequency of rotation of the working chamber of the mixer-activator from 80 to 90 min^{-1} is sufficient to destroy agglomerates and distribute CNTs in a metal matrix (Figure 2). In this case, the amount of energy supplied makes it possible to preserve the structure of the dendritic particles of the copper matrix.

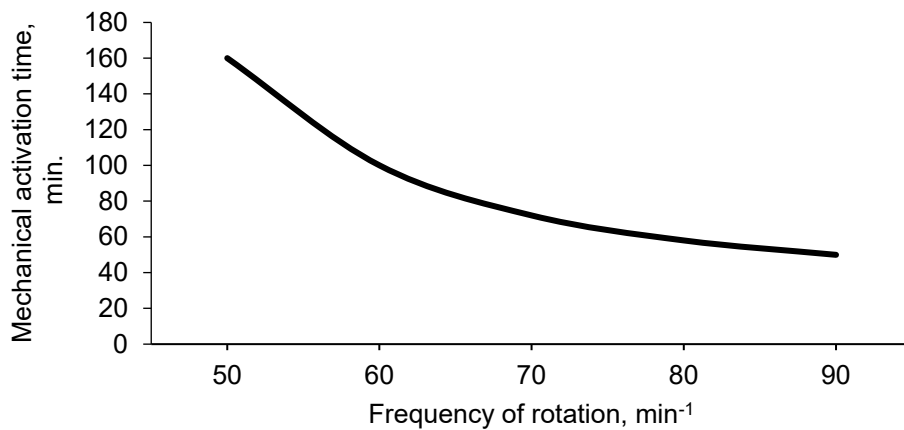


Fig 2. Dependence of mechanical activation time on the frequency of rotation of the working chamber of the mixer-activator

Thus, when processing composite materials based on powder systems “copper – nanostructured filler” in the mixer-activator, simultaneous processes of destruction and reduction in the size of agglomerates of carbon nanostructures, distribution and fixation of filler nanoparticles in the surface layer and in the interdendritic space of powder particles of the metal matrix occur, which ultimately ensures an increase in the number of metal-to-metal contacts.

3. Conclusions

A mathematical model of the process of mechanical activation of a powder mixture based on a metal matrix and carbon nanostructures has been developed. This model takes into account the processes of van der Waals interaction of carbon nanostructures, as well as the shape, dimensions, and physical and mechanical properties of the initial dispersed components of various structural levels, technological parameters of mechanical activation, and design features of the working chamber of the mixer-activator. The mathematical model, taking into account the criteria for the effective separation of agglomerates of carbon nanostructures and their distribution in the process of mixing nano- and micro-sized initial components of composite materials, makes it possible to determine the energy values of the van der Waals interaction of

carbon nanostructures, the energy values supplied by the mixer-activator at given technological parameters of mechanical activation, and also to predict the optimal time of mechanical activation of a powder system of various masses, sufficient for the destruction of agglomerates of carbon nanostructures and their distribution in a powder metal matrix.

Using the developed mathematical model, it was found that for a composite system based on a copper matrix filled with 0.07 wt. % of CNTs, the amount of mechanical energy supplied over a period of 55 to 60 min at a rotational speed of the working chamber of the mixer-activator from 80 to 90 min⁻¹ is sufficient to destroy agglomerates and distribute CNTs in a metal matrix.

References

1. Chung D.D.L. Composite materials. Berlin, Springer, 2010, 368 p.
2. Hutchings I., Shipway Ph. Tribology: friction and wear of engineering materials. Oxford, Butterworth-Heinemann, 2017, 412 p.
3. Pasovets V. N., Kovtun V. A., Pleskachevskiy Yu. M. Production, properties and safety of composites based on powder metals and carbon nanostructures. Gomel, BelGUT, 2011, 200 p.
4. Kovtun V., Pasovets V., Mirchev Y., Mihovski M. Research of the interaction energy of carbon nanotubes in the agglomeration process. International journal “NDT Days”, 2022, vol. 3, iss. 2, pp. 72–79.
5. Hamaker H. C. The London van der Waals attraction between spherical particles. Physica, 1937, vol. 4, iss. 10, pp. 1058–1072.
6. Israelachvili J.N. Intermolecular and surface forces. London, Academic Press, 1992, 704 p.
7. Bhushan B., Fuchs H., Tomitori M. Applied scanning probe methods viii: scanning probe microscopy techniques. Berlin, Springer-Verlag, 2008, 519 p.
8. Huang Y.Y., Terentjev E.M. Dispersion of carbon nanotubes: mixing, sonication, stabilization, and composite properties. Polymers, 2012, vol. 4, no 1, pp. 275–295.
9. Kovtun V., Pasovets V. Carbon nanostructures introduction into powder micro-sized copper matrix. 1st International Architectural Sciences and Application Symposium, Ankara, 27 – 29 October 2021; ed.: A. Gul, O. Demirel, S. Seydosoglu. Isparta, ISPEC Publishing House, 2021, pp. 588 – 596.
10. Kovtun V., Pasovets V. Mixer-activator. Patent BY 8201. Publ. 30.04.2012.