MACROKINETICS OF STRUCTURAL AND CHEMICAL TRANSFORMATIONS IN A BINARY POWDER MIXTURE AFTER MECHANICAL TREATMENT

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One of the effective methods for accelerating chemical transformations in powder mixtures is intense mechanical treatment [1 - 4]. Planetary mills are most often used for this purpose in practice. After mechanical treatment, along with the grinding of powders, there is the formation of an interphase surface to initiate chemical interactions. The interphase surface is formed by «spreading» one of the reagents on the other in the place of frictional contact. During mechanical treatment, there is the continuous grinding of such layered structures (microcomposites) and the formation of new composites with a more complex internal structure, in which reaction products can appear. The development of this process reduces the size of separate layers of reacting substances, namely the scale of heterogeneity that determines the characteristic time of mass transfer of reactants towards each other [5].

Simultaneously with the grinding and formation of microcomposites, additional structural defects are created in the components of the mixture, where excess energy is accumulated, in contrast to the untreated material. In the macroscopic approximation, the some proportion of this energy reduces the activation barrier of chemical interaction. Depending on the intensity and time of mechanical treatment, chemical transformations can occur in the mill.

The purpose of this paper is to construct a mathematical model in the macroscopic approximation for the mechanical treatment of a binary mixture considering the formation of mechanocomposites to estimate the kinetics of chemical transformations.

The dynamics of the mechanical treatment of the powder mixture is described by the equations as follows: grinding, change in the relative volumes of components during agglomeration, change in the interphase surface in mechanocomposites, chemical transformations, the rate of excess energy in the reagents and the reaction product.

The dynamics of chemical and structural transformations in mechanocomposites is numerically studied during mechanical treatment. The results have shown that even after the grinding limit is reached and the size of the particles and the external surface area are practically not changed, the internal structure becomes more complicated, and the magnitude of the interphase surface and the uniform distribution of the components in the mechanocomposites are increased. This structure evolution of the mechanically processed powder mixture is in qualitative agreement with the experimental data given in [6, 7] and with the papers cited in these works.

Depending on the control parameters, the application areas of different modes are determined for the mechanical treatment of the powder mixture. Analytic relations are obtained for estimating the parameters of the layered structure of mechanocomposites, the degree of activation and the fraction of the converted substance.

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