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Predictive Model for Determining the Dispersion Component of Surface Free Energy in Dispersion-Filled Polymer Composites

DANCHENKO Yuliya[1,a*], ANDRONOV Vladimir[1,b], KARIEV Artem[2,c], MIRUS Oleksandr[4,d] and KULAKOV Oleg[3,e]

[1]National Academy of the National Guard of Ukraine, 3, Zakhysnykiv Ukrainy sq., Kharkiv, 61001, Ukraine

[2]National Technical University «Kharkiv Polytechnic Institute», 2, Kyrpychova str., Kharkiv, 61002, Ukraine

[3]National University of Civil Defense of Ukraine, 94, Chernyshevska str., Kharkiv, 61023, Ukraine

[4]Lviv State University of Life Safety, 35, Kleparivska str, Lviv, 79007, Ukraine

[a]u_danchenko@ukr.net, [b]va_andronov@ukr.net, [c]artem.karev@khpi.edu.ua, [d]mirus@ukr.net, [e]kulakov_oleh@nuczu.edu.ua

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Abstract. The paper develops a predictive model to determine the influence of the value of the dispersion component of the free surface energy (FSE) and the volume fraction of fillers on the dispersion component of the FSE of a polymer composite. Mathematical equations and graphical relationships illustrating these relationships are presented. The model is based on the assumption that in composites the FSE value is partially determined by interactions at the polymer-filler interface. Using the predictive model, it was established that the dispersion component of the free surface energy (FSE) can be a reflection of the properties of polymer composites. The reliability of the predictive assessment is shown on the example of an epoxy polymer composite with various mineral fillers.

Introduction

Surface energy characteristics are a reflection and consequence of internal chemical and physicochemical processes that occur during the formation of any, including polymer composites. In the formation of the energy characteristics of the surface of filled polymer composites, not only the chemical and physicochemical processes of polymer formation play a major role, but also interactions at the polymer-filler interface (interphase interactions). The energy state of a solid surface is characterized by the value of the free surface energy (FSE), which can be a criterion for assessing many protective and operational properties of polymer composites. The value of FSE includes dispersion and acid-base components, which reflect the nature of interactions during the formation of a solid, including polymer composites. The determination of the FSE value is mostly based on experimental measurements of contact angles of wetting of a solid surface by liquids with different surface tension and polarity and involves a large number of experimental studies. Therefore, the ability to predict the values of the FSE components of filled polymer composites is an important theoretical and practical problem. The task of this study is to predict the dispersion component of the FSE of polymer composites filled with dispersed fillers.

Characterization of Surface Free Energy Components of Filled Polymer Composites

The free surface energy (FSE) of a solid surface is characterized by the uncompensated surface energy at the solid–gas interface. According to Fawkes theory [1,2], the FSE (γ_s) of any solid surface is expressed as the sum of components, each of which reflects the nature of interactions in the solid: