Таблица 2. Физико-химические свойства эпоксидных композитов

Состав композиции, масс.ч., отвержденной 15 масс.ч. ПЭПА	$T_н$, ^oC	$T_к$ ^0C	Выход карбонизованных структур при $T_к$, % масс.	$T_в$, ^0C
100ЭД-20	200	390	40 (390 ^0C)	86
100ЭД-20+40ТХЭФ	180	360	55 (360 ^0C)	100
100ЭД-20+40ТХЭФ+0.05Al_2O_3	180	365	50 (365 ^0C)	122

Примечание: $T_н$, $T_к$ – начальная и конечная температура основной стадии термолиза; $T_в$ – теплостойкость по Вика.

ЛИТЕРАТУРА

1. Осипов П.В., Осипчик В.С., Смотрова С.А., Савельев Д.Н. Регулирование свойств наполненных эпоксидных олигомеров // Пластические массы. – 2011. - № 4 – С. 3-5.
2. Мостовой А.С. Использование эпоксисиланов при создании эпоксидных композитов с повышенными физико-химическими и механическими свойствами // Перспективные материалы. – 2016. – № 4. – С. 60-66.
3. Мостовой А.С., Яковлев Е.А., Бурмистров И.Н., Панова Л.Г. Использование модифицированных наноразмерных частиц полититаната калия и физических методов модификации эпоксидных составов с целью повышения их эксплуатационных свойств // Журнал прикладной химии. – 2015. – Т. 88, № 1. – С. 138-149.
4. Мостовой А.С., Панова Л.Г., Курбатова Е.А. Модификация эпоксидных полимеров кремнийсодержащим наполнителем с целью повышения эксплуатационных свойств // Вопросы материаловедения. – 2016. – № 2 (86). – С. 87-95.

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CALCULATION OF THE TOTAL ENERGY OF SnO_2 FRAGMENT OF STRUCTURE USING NWCHEM SOFTWARE

Quantum-mechanical characteristics of electrons and their behavior in general determine the total energy of the quantum system. Description of the behavior of electrons in a multi-electron system is somewhat difficult, since in such a system there are different types of interactions: exchange, exchange-correlation, etc. Thus, some approximations and simplifications

are used in the process of solving the basic quantum-mechanical equation – the Schrödinger equation.

In practice, the Density Functional Theory (DFT) is often used to describe multi-electronic systems. This method is universal and applicable to both electronic gases and multi-electron condensed systems. DFT is based on the following principles: the energy of the ground state of the system of interacting particles in this external field is represented as a single functional, which depends only on the electron density of the particles [1]. Since the movement of electrons in the condensed state is strongly correlated, a model system of non-interacting particles in which the total energy and electron density coincide with similar functions of the real system is used to describe such a system [2].

The main purpose of density functional theory is to replace the multi-electron wave function with electron density function. This allows to simplify the problem significantly, since the multi-electron wave function depends on several variables, while the density is a function of only three spatial coordinates [3].

Calculation of the total energy of a system, which is a solid crystalline body – the 49-atoms SnO_2 cluster (Fig. 1) was done in NWChem software using the mentioned above non-empirical method – density functional theory (DFT).

NWChem is free and open-source software distributed under the terms of the Educational Community License (ECL) 2.0. This software provides a wide range of empirical, non-empirical and hybrid methods of computational chemistry implemented as separate modules. The main advantages of NWChem compared to other computational chemistry software (e.g. MOPAC, GAMESS-US, Gaussian) is that NWChem has open source code, implements almost all of computational chemistry methods, supports multiprocessor systems and high-performance clusters through MPI, has wide configuration capabilities, simple structure of input files and is updated and improved regularly. The quantity and quality of documentation covering all the functionality of the software is also worth mentioning [4,5].

The total DFT energy was calculated in direct mode using the B3LYP hybrid exchange-correlation functional which consists of Hartree-Fock (Exact) Exchange, Slater Exchange Functional, Becke 1988 Exchange Functional, Lee-Yang-Parr Correlation Functional, VWN I RPA Correlation Functional. A 3-21G basis set was chosen for the optimal ratio of calculation time and accuracy. The calculated total energy was -56982.3035569 Hartree. The total energy consisted of following components (Hartree): one electron energy = -144067.75663, coulomb

energy = 56094.44348, exchange-Corr. Energy = -1788.31012, nuclear repulsion energy = 32779.31971.

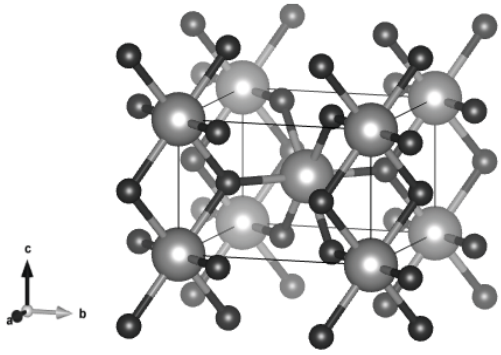

Fig. 1. The 49-atom SnO_2 cluster.

The approximate accuracy of numerical integration used to estimate the exchange-correlation contribution to the density functional was $1x10^{-5}$. Since the calculations were performed iteratively, the main convergence criteria of calculations was the energy difference between the two iterations – less than $5x10^{-6}$.

ЛИТЕРАТУРА

1.http://lms.physics.spbstu.ru/pluginfile.php/689/mod_resource/content/4/QTMPS_Part_02.pdf.
2. https://kau.org.ua/images/Romanskiy.pdf.
3. Сатанин, А.М. Введение в теорию функционала плотности / А.М. Сатанин. Нижний Новгород, 2009.
4.Valiev M., Bylaska E.J., Govind N., et al., "NWChem: a comprehensive and scalable open-source solution for large scale molecular simulations" Comput. Phys. Commun. 181, 1477 (2010), doi:10.1016/j.cpc.2010.04.018.
5. https://github.com/nwchemgit/nwchem/wiki.

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АНАЛИЗ КИСЛОТНО ОСНОВНЫХ СВОЙСТВ НАНОКОМПОЗИТА НА ОСНОВЕ АКТИВИРОВАНОГО УГЛЯ

Среди сорбционных материалов, которые обладают большой удельной поверхностью и достаточно высокими сорбционными свойствами, наиболее известными являются активированные угли.