



Russian Science Foundation



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Время/Дата	Воскресенье 29.09.2024	
	Прибытие и заселение участников	
	Понедельник 30.09.2024	
09.00 – 09:30	Утренний кофе, регистрация	
09:30 – 09:50	Открытие Школы, презентация треков	
09:50 – 10:35	Лекция 1. Биомиметические материалы и технологии биопечати для формирования эквивалентов органов и тканей (лектор – Федор Сенатов , НИТУ МИСИС)	
10:35 – 11:20	Лекция 2. Получение и модификация наночастиц оксидов железа для биомедицины (лектор — Алексей Никитин , НИТУ МИСИС)	
11:20 – 12:00	Лекция 3. FDM и DIW печать композитами на основе PVDF/PLA и магнитных наночастиц (лектор – Петр Ершов , БФУ им. И. Канта)	
12:00 – 12:40	Обед	
12:40 – 13:30	Тур по лабораториям НОЦ «Умные материалы и Биомедицинские приложения»	
13:30 – 14:45	Лекция 4. Как подаваться на акселлераторы. Подготовка результатов работы к подаче на финансирование (лектор – Никита Востров , ТвГУ)	
14:45 – 16:00	Практика	
16:00 – 16:30	Кофе-пауза	
16:30 – 18:30	Практика	
18:30 – 20:00	Фуршет. Интерактивная игра на знакомство.	

	Вторник 01.10.2024	
09.00 – 09:30	Утренний кофе	
09:30 – 10:10	Лекция 1. Магнитные и магнитоэлектрические нанокомпозиты. Мессбауэровские исследования (лектор – Александр Камзин , ФТИ им. А.Ф. Иоффе)	
10:10 – 10:50	Лекция 2. Проектирование персонализированных аддитивно изготовленных биомедицинских изделий с управляемой морфологией (лектор — Михаил Ташкинов , ПНИПУ)	
10:50 – 11:35	Доклад 1. Разработка магнитоэлектрического композита с увеличенным содержанием бета фазы и однородным распределением наночастиц в матрице PVDF (докладчик − Павел Воронцов, БФУ им. И. Канта) Доклад 2. Влияние количества нанонаполнителя феррита кобальта СоFe ₂ O ₄ на формирование электроактивной фазы в матрице композитов на основе полимера ПВДФ (докладчик − Станислав Воронцов, БФУ им. И. Канта) Доклад 3. Использование аддитивных технологий для изготовления умных материалов (докладчик − Егор Сергеев, БФУ им. И. Канта)	
11:35 – 12:10	Обед	
12:10 – 13:40	Лекция 3. Обменносвязанные композиты для производства постоянных магнитов (лектор – Дмитрий Карпенков , НИТУ МИСИС)	
13:40 – 16:00	Практика	
16:00 – 16:30	Кофе-пауза	
16:30 – 17:30	Лекция 4. Что такое и чем занимаются центры трансфера технологий (лектор — Константин Астанков , ИТМО)	
17:30 – 18:30	Консультации/практика	

	Среда 02.10.2024	
9:00 – 9:30	Утренний кофе	
9:30 – 10:10	Лекция 1. Моделирование магнитоактивных эластомеров (лектор — Олег Столбов , ИМСС УрО РАН)	
10:10 – 10:50	Лекция 2. Введение в магнетизм частиц (онлайн, лектор – Александр Омельянчик , БФУ им. И. Канта)	
10:50 – 11:35	Лекция 3. Вращательный гистерезис системы однодоменных магнитных частиц и магнитная восприимчивость (лектор — Лариса Панина , НИТУ МИСИС)	
11:35 – 12:20	Лекция 4. Печать пьезополимерами (лектор – Никита Востров , ТвГУ)	
12:20 – 13:00	Обед	
13:00 – 14:15	Лекция 5. Оформление и защита результатов деятельности (лектор – Андрей Николаев , ИТМО)	
14:15 – 16:00	Практика	
16:00 – 16:30	Кофе-пауза	
16:30 – 18:00	Практика	
18:00 – 19:00	Консультации/практика	

	Четверг 03.10.2024	
9:00 – 9:30	Утренний кофе	
9:30 – 10:10	Лекция 1. Магнитные, пьезо- и магнитоэлектрические наноматериалы и скэффолды для решения современных задач биологии и медицины (онлайн, лектор — Роман Сурменев , ТПУ)	
10:10 – 10:50	Lecture 2. An Overview of Density Functional Theory: Methods and Characterization Techniques for Researchers (lector – Niaz Schanaver, Thal University Bhakkar)	
10:50 – 11:30	Лекция 3. Поиск оптимальной структуры соединений для увеличения ширины запрещенной зоны: подходы USPEX и VASP (лектор – Курбан Магомедов , БФУ им. И. Канта)	
11:30 – 12:15	Доклад 1. Возбуждение магнитных и упругих колебаний в кристаллах марганцево-цинковой шпинели, включая переходную область спиновой переориентации (докладчик — Михаил Майбуров, СГУ им. Питирима Сорокина) Доклад 2. Размерный эффект в магнитооптических спектрах наноструктур (докладчик — Марина Симдянова, МГУ имени М.В. Ломоносова) Доклад 3. Применение функционализированных магнитных наночастиц для детектирования нуклеиновых кислот (докладчик — Дарья Горбенко, ИТМО)	
12:15 – 13:00	Обед	
13:00 – 16:00	Практика	
16:00 – 16:30	Кофе-пауза	
16:30 – 18:00	Лекция 4. Мастер-класс «Секреты построения эффективной питч- презентации» (лектор — Андрей Цымбал , НИУ ВШЭ)	
18:00 – 20:00	Фуршет	

	Пятница 04.10.2024	
9:00 – 9:30	Утренний кофе	
9:30 – 10:30	Лекция 1. Полимерные бионические актуаторы для мягкой робототехники (лектор – Алексей Максимкин , МГМУ им. И.М. Сеченова)	
10:30 – 11:30	Доклад 1. Выбор покрытия частиц для усиления магнитоэлектрического эффекта в композитах на основе ПВДФ (докладчик — Виталий Сальников, БФУ им. И. Канта) Доклад 2. Влияние магнитоэлектрической стимуляции нанокомпозитов на основе PVDF на активность мезенхимальных стволовых клеток (докладчик — Екатерина Корепанова, БФУ им. И. Канта) Доклад 3. Перспектива использования аддитивных технологий для изготовления микромагнитных структур из порошковых материалов сплавов Fe-TM-Nd-REM-B, полученных методом закалки расплава распылением расплавленного газа (докладчик — Игорь Пастухов, БФУ им. И. Канта) Доклад 4. Механические свойства волоконных композитов с климаторегулирующим эффектом (докладчик — Борис Прядезников, БФУ им. И. Канта)	
11:30 – 12:10	Лекция 2. Как заработать на инженерных знаниях (лектор – Александр Енин , генеральный директор ООО КБ «ЮЖНЫЙ»)	
12:10 – 13:00	Обед	
13:00 – 15:30	Практика/Консультации/Подготовка к защите проектов	
15:30 – 16:00	Кофе-пауза	
16:00 – 17:30	Выступление групп с питчами. Лучшим – приз!	
17:30 – 18:30	Практика/Консультации/Подготовка к защите проектов	

	Суббота 05.10.2024	
10:00 – 11:00	Утренний кофе и стендовая секция	
11:00 – 11:45	Лекция 1. Суперконструкционные полимеры и композитные материалы на их основе для 3D печати. Исследование термических свойств полимерных материалов (лектор — Азамат Жанситов , КБГУ им. Х.М. Бербекова)	
11:45 – 13:00	Защиты проектов	
13:00 – 13:30	Закрытие Школы	

Стендовые доклады:

- 1. Разработка системы высокоточного картирования механических напряжений (**Николай Шилов**, БФУ им. И. Канта)
- 2. Улучшение межфазного взаимодействия в нанокомпозитах C₆₀/PVDF путем трифторметилирования (**Денис Петрухин**, БФУ им. И. Канта)
- 3. Влияние магнитной стимуляции нанокомпозитов на основе PVDF на активность минерализации мезенхимальных стволовых клеток (Виолетта Фролова, БФУ им. И. Канта)
- 4. Измерение пьезоэлектрической константы d33 композитных материалов (Артем Игнатов, БФУ им. И. Канта)
- 5. Исследование композитных микродисков для применения в биомедицине (**Анна Моторжина**, БФУ им. И. Канта)
- 6. Изготовление и исследование композитных систем на основе ферромагнитных микропроводов (Валерия Колесникова, БФУ им. И. Канта)
- 7. Магнитный отклик и зарождение фракталоподобных агрегатов (**Екатерина Чемезова**, УрФУ им. Б.Н. Ельцина)
- 8. Магнитный отклик многоядерных частиц с различной микроструктурой: роль межчастичных взаимодействий (**Елена Грохотова**, УрФУ им. Б.Н. Ельцина)
- 9. Установка для магнитомеханического разрушения клеток (**Дания Зиннятуллина, Исрафиль Шаманов**, БФУ им. И. Канта)
- 10. Магнитные и магнитооптические свойства одномерных магнитоплазмонных кристаллов с нарушенной зеркальной симметрией (**Зоя Григорьева**, БФУ им. И. Канта)
- 11. Магнитно-функционализированные композиты MXene для сорбции тяжелых металлов: Cu(II), Pb(II) и Fe(III) (**Курбан Магомедов**, БФУ им. И. Канта)

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Oral Talks

Application of functionalized magnetic nanoparticles for detection of nucleic acids

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Early diagnosis of diseases is essential for effective treatment and can be life-saving for patients. There are various methods for quickly identifying pathogens, with PCR being the gold standard. However, PCR necessitates costly equipment and highly trained personnel, leading to significant expenses. DNA nanosensors represent a rapidly advancing technology that could serve as a cost-effective alternative to existing methods, enhancing the efficiency of the diagnostic process.

A DNA nanosensor with a four-way junction structure was designed for the malB gene of E.coli. The universal molecular beacon was immobilized on the surface of magnetic nanoparticles using amide and streptavidin-biotin interactions, the immobilization reactions were then confirmed by IR spectroscopy and fluorescence analysis.

A method was developed to determine the yield of immobilization reactions using deoxyribozyme 10-23, the yield of immobilization reactions via amide interactions was 0.2%. The hypothesis was tested that as the number of bound universal molecular beacon on each nanoparticle decreased, the sensitivity limit of the sedimentation test would also decrease.

The sensitivity limit decreased to 1 uM of analyte when nanoparticles modified with fewer beacons were used. To increase the sensitivity of the sedimentation test, one of the sensor strands was split into two, the efficiency in recognizing different single nucleotide substitutions in the analyte was shown by performing calculations in NUPACK as well as hybridization with fluorescent universal molecular beacon.

In the case of the sedimentation test, the system was selective to one of the substituents, with a selectivity factor of 82.7%. The sedimentation test system was also sensitive to the LAMP amplicon of the malB gene.

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Excitation of magnetic and elastic oscillations in manganese-zinc spinel crystals including the spin reorientation transition region

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Nonlinear magnetoelastic dynamics of films and plates in the area of spin-reorientation phase transitions (SRPT) is currently attracting significant attention from researchers [1]. The variety of magnetic oscillation modes in magnetic plates and films allows them to be used in nonlinear frequency conversion devices, ultra-sensitive magnetic field sensors, as well as absorbers of electromagnetic fields, acoustic vibrations, and waves [2-4]. However, many of the nonlinear effects associated with the crystalline structure of solids, especially in the region of magnetic phase transitions, are still poorly understood [1].

In the present work, we computed the amplitudes of magnetic and elastic oscillation components of plates made from manganese-zinc spinel (MZS) with the composition Mn_{0.61}Zn_{0.35}Fe_{2.04}O₄ under the influence of an alternating magnetic field. The choice of MZS crystal as the object of study was explained by the observation of the inversion of the sign of the first magnetic anisotropy constant K1 in a zero constant magnetic field with changing temperature [4, 5]. In this study, we calculated the amplitudes of magnetic and elastic oscillations based on solving a system of ordinary differential equations for magnetic and elastic dynamics [6]. It was assumed that the total energy density of the crystalline plate is equal to the sum of the densities of magnetic, elastic, and magnetoelastic energy [4]. We obtained temperature dependencies of the components of the magnetization vector mx,y and elastic displacement ux,y for the MZS plate at various values of the constant magnetic field. The obtained temperature dependencies showed that near zero values of K1, the amplitudes of magnetic and elastic oscillations are infinitesimally small, mx,y ~10-8 and ux,y ~10-16 cm. Narrow peaks were found in the temperature curves of the magnetic components mx, y(T), attributed to ferromagnetic resonance (FMR), which are absent in this temperature range for the elastic displacement amplitude ux,y(T). The behavior of the elastic component amplitudes ux, y is characterized by their increase with decreasing temperature due to the increase of |K1| until maximum values are reached for the magnetization components, after which they transition to a constant value.

The research was supported by a grant from the Russian Science Foundation (project No. 21-72-20048).

- [1] Kotov L.N., Physics of the Solid State 60, 1153 (2018)
- [2] Vlasov V.S., Bull. Russ. Acad. Sci. Phys. 77, 1255 (2013)
- [3] Vlasov V.S., J. Commun. Technol. Electron. 59, 441 (2014)

- [4] Pleshev D.A., Bull. Russ. Acad. Sci. Phys. 83, 901 (2019)
- [5] Vlasov V.S., J. Commun. Technol. Electron. 54, 821 (2009)
- [6] Vlasov V.S., Acoustical Physics 68, 18 (2022)

Effect of the amount of CoFe₂O₄ cobalt ferrite nanofiller on the formation of electroactive phase in the matrix of PVDF polymer-based composites

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This work investigates the effect of different amounts of CoFe₂O₄ (cobalt ferrite) nanofiller on the formation of the electroactive phase in polyvinylidene fluoride (PVDF)-based composites. Cobalt ferrite is known for its excellent magnetic and electrical properties [1], making it a promising candidate for enhancing the performance of PVDF-based composites in applications such as sensors, actuators, and energy storage devices [2].

The composites were synthesized with different weight percentages of $CoFe_2O_4$, ranging from 5% to 15%, and characterized using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM) to analyze the structural and morphological changes. The electroactive phase of PVDF, primarily the β -phase, was evaluated by differential scanning calorimetry (DSC).

The results show a significant correlation between the CoFe₂O₄ concentration and the crystallization behavior of PVDF. An optimum loading of 10% CoFe₂O₄ was found to enhance the formation of β -phase, resulting in improved dielectric and piezoelectric properties. Above this threshold, excessive nanofiller content led to agglomeration, which negatively affected the development of the electroactive phase.

This study provides valuable insights into the development of PVDF-based composites with tunable electroactive properties, highlighting the critical role of cobalt ferrite nanofillers in optimizing the performance of polymer composites for advanced technological applications.

- [1] Boosting Magnetoelectric Effect in Polymer-Based Nanocomposites; A. Omelyanchik, V. Antipova, C. Gritsenko, V. Kolesnikova, D. Murzin, Y. Han, A. V. Turutin, I. V. Kubasov, A. M. Kislyuk, T. S. Ilina, D. A. Kiselev, M. I. Voronova, M. D. Malinkovich, Y. N. Parkhomenko, M. Silibin, E. N. Kozlova, D. Peddis, K. Levada, L. Makarova, A. Amirov, and V. Rodionova; Nanomaterials; DOI: 10.3390/nano11051154.
- [2] CoFe2O4 nanofiller effect on β -phase formation of PVDF matrix for polymer-based magnetoelectric composites; Choi, Moon, Yang, Su-Chul; Materials Letters; DOI:10.1016/j.matlet.2018.04.024.

The prospect of using additive technologies for the production of micromagnetic structures from powder materials of Fe-TM-Nd-REM-B alloys obtained by melt quenching thawed gas atomization.

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Using powder materials of multicomponent alloys of the Fe-TM-Nd-REM-B system, where Nd+REM=32÷35 and B=1.08÷1.23 wt. %, which were obtained by spraying a melt jet with an inert gas stream in a special quenching atmosphere (MQGAP - Melt Quenching Gas Atomization Powder's) and using the domestic small-sized laser technological installation MUL-1-M-150 in the micro-melting mode in an inert flowing atmosphere, the principal possibility of forming a magnetic alloy with appropriate functional properties in volume has been experimentally shown a single initial powder (up to 500 microns) or powder surfacing (more than 1 mm) on a metal substrate. The results obtained will be used to form point, linear and micro-volumetric magnetic systems for general and special purposes. In particular, a linear micromagnetic system will be used to form a concentrated local magnetic field for a flaw detector of micromagnetic releases of martensite or ferrite in the weld material of stainless steel and heat-resistant austenitic alloys.

Comprehensive studies of the influence of chemical and fractional compositions on the structural and phase state of the alloy and the functional properties of the deposited magnetic material have been carried out. The studies were performed using metallographic (SIAMS 800, including OLYMPUS BX-51 microscope and SIAMS Drive System), X-ray fluorescence energy dispersion (CEP 01 Elvax), X-ray diffraction (DRONE-3-M), scanning electron microscopic (SEM JEOL JSM-6390LV), magnetometric (ATE-8702) analyses, X-ray tomography (Y.Cheetah microfocus X-ray system from YXLON) and microhardness measurements (PMT-3M and SHIMADZU HMV G21ST).

The effect of isothermal annealing on the change in the structural and phase state in the IQGAP alloy has been studied. It is shown that isothermal annealing is accompanied by structural and phase changes affecting the weighted average grain size and morphology of Fe14Nd2B. At the same time, the obtained qualitative and quantitative dependences indicate that the recrystallization of the grains of the main magnetic phase proceeds in the alloy by mechanisms that are determined by more complex processes of heat and mass transfer than stationary processes of diffusion transfer of atomic components of the alloy. It is assumed that the unsteady flow of liquid triple eutectic along the intergranular layer can be realized in IQGAP, as in a developed closed capillary system.

Taking into account the revealed patterns, it is proposed to vary the initial state of MQGAP (different chemical and fractional compositions, different annealing of the initial

powder) and the temperature of the substrate for laser surfacing of the Fe-TM-Nd-REM-B alloy powder material during laser surfacing.

The research was carried out at the expense of the grant of the Russian Science Foundation No. 22-19-20157 (https://rscf.ru/project/22-19-20157/) and the grant in the form of a subsidy from the budget of the Kaliningrad region No. 11-C/2024.

CHOICE OF COATINGS TO ENHANCE THE MAGNETOELECTRIC EFFECT IN PVDF-BASED COMPOSITES

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Current research is aimed at improving the magnetoelectric efficiency of polymer-based composites with multiferroics, one of the promising ways being increasing the mechanical coupling between the ferromagnetic and ferroelectric parts of the composite [1]. This paper shows the changes in the phase composition and mechanical properties of PVDF-based composites as a result of coating CoFe2O4 nanoparticles with one of the following compounds: oleylamine (OAm), polyethyleneglycol (PEG), oleic acid (OA), and citric acid (CA) to increase the voltage coefficient (α ME) of the magnetoelectric effect. Coating with OAm or PEG makes it possible to increase the α ME value from \sim 17 mV/ cm Oe for the composite with bare nanoparticles to \sim 30 and 38 mV/ cm Oe , respectively (Fig. 1).

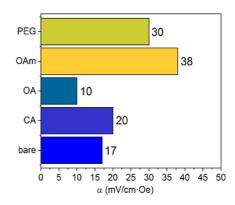


Figure 1. Maximum ME stress coefficient (αME) for polymer composites after stretching.

This study was supported by the Russian Science Foundation grant No. 21-72-30032.

Literature:

[1] Omelyanchik A . et al . Boosting magnetoelectric effect in polymer-based nanocomposites // Nanomaterials. $-2021.-T.\ 11.-No.\ 5.-S.\ 1154.$

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Size-effect in magneto-optical spectra of nanostructures

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Annotation. In this work, within the framework of the effective medium method, we study the influence of various microscopic parameters, semi-classical and quantum size effects on the magneto-optical spectra of the equatorial Kerr effect of magnetic nanocomposites (CoFeB)_x(LiNbO₃)_{1-x} and two-layer NiFe/Ta structures. The calculations took into account the possibility of spin-orbit interaction enhancement in a thin near-surface layer, which affects both interband and intraband optical transitions.

Keywords: nanostructures, magneto-optics, size effect.

Magneto-optical (MO) spectroscopy, based on measurements of the spectral dependences of the equatorial Kerr effect, also called the transverse Kerr effect (TKE), allows to obtain information about their electronic, crystalline and magnetic microstructure without contact and during the deposition of thin-film samples [1]. In this case, the measured parameter TKE, $\delta(\omega)$), namely the relative change in the intensity of p-polarized light during magnetization of samples, is complexly related to their optical and MO properties. Therefore, the inverse problem arises of reconstructing microscopic parameters from measurements of spectral dependences of the TKE. In the case of magnetic nanostructures, such as magnetic nanocomposites or multilayers, this task is significantly complicated by the presence of quasi-classical and quantum dimensional effects, and various possible types of spin-orbit interaction (SOI) on the interface of layers or on the surface of nanoparticles. The latter factor is the most important, since MO effects are determined by the action of SOI, which differ significantly in volume and on the surface of nanoparticles. In this work, the influence of various microscopic parameters, quasi-classical and quantum dimensional effects on the spectra of ferromagnetic metal-dielectric nanocomposites is investigated within the framework of the effective medium method, (CoFeB)_x(LiNbO₃)_{1-x} with different volume concentrations of the magnetic component, including near the percolation threshold, and twolayer structures of NiFe/Ta. The calculation method is described in detail in [2]. Additionally, we took into account the possibility of amplification of owls in a thin near-surface layer with a thickness of, which affects both interband and intraband optical transitions. As an example, Fig.1 and Fig.2 show the calculated spectra of the nanocomposite (Co)_{0.35}(SiO₂)_{0.65} at different values of the ratio of the parameters of the CO in the surface layer and in the volume λs/λb and at different values of the thickness of the surface layer, and with parameters different from the volume. As can be seen from these drawings, the SOV in the surface layer critically affects the TKE spectra up to a sign change.

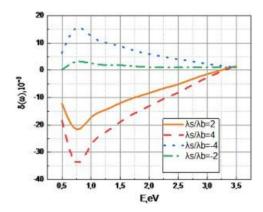


Fig.1. Calculated spectra of the TKE nanocomposite (Co)x(SiO2)1-x at x=0.35, with different values of the ratio of the parameters of the SOI in the surface layer and in the volume $\lambda s/\lambda b$: 2 (solid line), 4 (dotted line), -4 (dots), -2 (dotted point). Parameters: plasma frequency, form factor L=0.3, granule size r=3 nm, surface layer thickness a/r=1/10

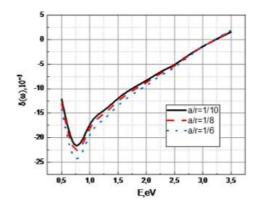


Fig.2. Calculated TCE spectra of nanocomposite (Co)x(SiO2)1-x at x=0.35 with different thicknesses of the a/r surface layer: 1/10 (solid line), 1/8 (dotted line), 1/6 (dots). Parameters: plasma frequency, form factor L=0.33, granule size r=3 nm, thickness of the surface layer a/r=1/10, the ratio of the parameters of the SOI in the surface layer and in the volume $\lambda s/\lambda b=2$.

The developed program makes it possible to identify the influence of each of the microscopic parameters on the TKE spectrum and determine from comparison with the experiment the parameters characterizing the surface of granules or layers, in particular, to determine the value of the coefficient of the anomalous Hall effect on the surface of granules, which is not available by other methods.

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Direct Ink Writing 3D printing of Polyvinylidene fluoride with magnetic particles

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Polyvinylidene fluoride (PVDF) is a widely used polymer with piezoelectricity, pyroelectricity, and ferroelectricity properties, making it suitable for sensors, actuators, and energy harvesting devices [1]. Also, by adding magnetic particles, it is possible to transform PVDF into multiferroic material that exhibits more than one type of ferroic order, such as ferroelectricity, ferromagnetism, and ferroelasticity [2]. Furthermore, this kind of material can be utilized in 3D printing technology that extends the area of its applications.

Additive manufacturing, such as Direct Ink Writing (DIW), allows for accurate control of geometry and adjustment of printing parameters during fabrication. In this work, DIW was used to print $10x10 \times -0.05$ mm PVDF films with magnetic nanoparticles (SrFe₁₂O₁₉, CoFe₂O₄). To create the printing ink, PVDF powder was dissolved in dimethylformamide in a 1:6 ratio, and after that, to the volume, 10% of magnetic nanoparticles were added. Printing was carried out at a 100 °C temperature of the DIW printer heating bed; partial hardening of the samples was observed already 5 minutes after printing and drying out by a 300 °C hot air soldering gun. Shrinkage less than 10 times compared to the original layer height was observed. The piezoelectric properties of the film were measured using a D33 meter, yielding values of (6±1) pC/H, while the magnetoelectric measurements were recorded at (2±1) mV/Oe·cm.

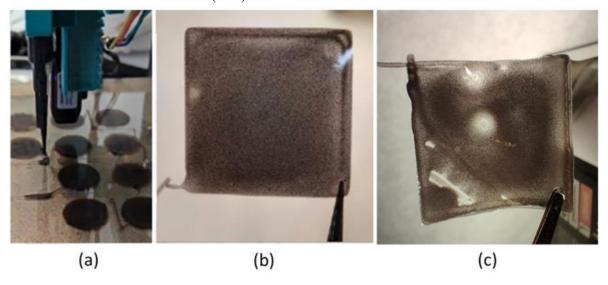


Figure 1. (a) A photo taken during the DIW printing process using PVDF/CFO ink; (b) Images of the printed PVDF/SrFe₁₂O₁₉ films without magnetic particle arrangement and (c) with out-of-plane magnetic particle arrangement.

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Moving forward, orienting magnetic particles using applied out-of-plane and in-plane configurations of the magnetic field during printing may allow for the precise arrangement of particles within the printed structure. This could lead to the fabrication of magnetoelectric multiferroic structures by spatially patterning the particles, with applications in sensors, actuators, and energy harvesters.

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Influence of magnetoelectric stimulation PVDF-based nanocomposites on mesenchymal stem cells activity

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Bone tissue treatment is a long and complex process with a high risk of complications that can negatively affect on quality of a patient's life. So, it's necessary to search for new effective methods for bone tissue regeneration. In bone tissue engineering increases interest in materials that are capable of influencing cellular behavior through electrical or magnetoelectric stimulation. One of the promising areas of bone tissue restoration is the development of biocompatible substrates with certain mechanical properties, such as strength, roughness, and piezoelectric response. These substrates promote proliferation and accelerated differentiation of stem cells in the osteogenic direction. Piezoelectric polymers have the ability to convert a mechanical voltage into an electrical pulse (direct piezoelectric effect) or an electrical pulse into a mechanical voltage (reverse piezoelectric effect). Such materials include the polymer polyvinylidene fluoride (PVDF), which has a high piezoelectric response and morpho-mechanical properties similar to those of bone tissue. The inclusion of nanoparticles in the piezopolymer matrix will activate the piezoelectric properties of PVDF due to stimulation by an alternating magnetic field.

In this work were two series of samples: PVDF films with 5% or 10% content of CoFe2O4 nanoparticles (PVDF+CFO). For biological studies, the samples were pre-sterilized (alcohol + UV radiation), after which they were attached to the bottom of culture plates. Plates with cells stimulated for 7 and 14 days. To assess proliferation of multipotent human mesenchymal stem cells (MMSCs) was used WST-1 assay. To assay activity of MMSC was used alkaline phosphatase. According to the results of work in wells with 5%PVDF+CFO samples with stimulation was a tendency of increasing proliferation. There was also a tendency of increasing agglomerations of cells with a high level of alkaline phosphatase, that may indirectly indicate the effect of magnetoelectric stimulation of PVDF+CFO nanocomposites on the activity of MMSCs.

This study demonstrates the potential of magnetoelectric stimulation of nanocomposites as a tool to increase cellular activity, which makes these materials potentially applicable for various biomedical applications.

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Figure 1. Representative images from fluorescence microscope of FetMSC well sites after 14 days of cultivation. The size scale is 50 microns. The cells in which alkaline phosphatase activity is observed are colored purple. Control – FetMSC cultivated without PVDF substrates.

Development of magnetoelectric composite with increased content of beta phase and homogeneous distribution of nanoparticles in PVDF matrix

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Polyvinylidene fluoride (PVDF) is a widely used polymer that has received considerable attention in various fields due to its high thermal stability, chemical resistance, ferro-, pyro-, and piezoelectric properties, which allow the material to be used in various applications such as electronics, biomedicine, etc. [1-3].

Building on the inherent properties of PVDF, researchers have explored the possibility of extending its capabilities by incorporating other materials. One of the most notable approaches is the inclusion of cobalt ferrite (CoFe2O4, CFO) magnetic nanoparticles (MNPs) as a filler. This combination results in a PVDF-based composite that exhibits both piezoelectric and magnetic properties, creating a multiferroic material. Such composites have expanded the applications of PVDFs, making them suitable for applications such as magnetic field sensors, transducers, multistage memory devices, and filters [4].

PVDF is a semi-crystalline polymer that can exist in at least four crystalline forms (α , β , γ , and δ), the formation of which is due to the different spatial arrangement of CH2 and CF2 groups [5,6]. Among them, β - and γ -phases have the strongest piezo- and ferroelectric properties [7,8]. The phase composition of PVDF can be controlled by various processing methods including heat treatment, cooling rate and addition of nucleating agents such as inorganic nanoparticles [9,10].

In the current era of technological progress, the study of functional materials is at the forefront of scientific innovation, paving the way for revolutionary developments in various fields such as biomedicine. Among such materials, magnetoelectric composites with magnetic and piezoelectric properties are particularly promising.

In this paper, magnetoelectric composites are studied, their synthesis is described and their characteristics are investigated. The composite material presented in this work consists of a piezoelectric polymer polyvinylidene fluoride (PVDF) and cobalt ferrite nanoparticles (CFO) embedded in its polymer matrix.

To realize this work, a protocol for the synthesis of magnetoelectric composites was investigated and optimized, considering factors such as preparation of PVDF and CFO, thickness of magnetoelectric composites, drying temperature and mixing time of PVDF-CFO

solution. The characteristics of the synthesized samples were characterized using techniques such as scanning electron microscopy (SEM), X-ray diffraction (XRD), atomic force microscopy (AFM), vibrating magnetometer (VSM), Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy (RAMAN) and differential scanning calorimetry (DSC) method. To describe the structural features of the composite in order to identify its potential functionalities.

The process of creating the magnetoelectric composite represents a key aspect of this research. In this work, we aim to take into account all the intricacies associated with the synthesis protocol, including the preparation of PVDF and CFO, the thickness of the films created, the drying temperature, the mixing time of the PVDF-CFO solution, and many other factors. Through rigorous research, we aim to explore all the nuances of component interactions, capturing factors that affect the properties and finished composite films.

In addition to the intricacies of synthesis, this research extends to the study of morphostructural characteristics of the composite.

Thus, this work aims to contribute to an emerging area of functional materials research, namely the application of magnetoelectric composites in biomedicine. Through the modernization of synthesis protocols, morphostructural analysis and biomedical research, we aim to unlock the multifaceted potential of PVDF-CFO composites.

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Effect of dynamic magnetic stimulation of PVDF-based nanocomposites on stem cell mineralization activity

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Bone injuries are regularly seen in a large number of people around the world. In many patients, bone regeneration after trauma is inappropriate or difficult due to the development of complications. To solve this problem, new therapies and materials capable of modulating cellular behavior and promoting tissue regeneration are being sought. The most interesting, in turn, are electroactive materials with properties similar to the extracellular matrix of bone tissue. Polyvinylidene fluoride (PVDF) is the most suitable material because of its biocompatibility and mechanical and piezoelectric properties similar to those of bone tissue [1]. This work proposes the use of magnetic stimulation of PVDF-based nanocomposites modified with magnetic CoFe₂O₄ nanoparticles to activate cell mineralization processes [2].

Biological validation of nanocomposites was performed on human mesenchymal stem cell line (FetMSC). Stimulation of cells cultured on the surface of nanocomposites and without was performed daily for 30 minutes. Cell viability was determined using WST-1 assay, measuring the optical density of the medium using a flatbed spectrophotometer. The activity of the mineralization process was assessed by staining with Alizarin red. Control measurements were carried out on 14 and 21 days of the experiment.

It was found that long-term incubation of stem cells on the surface of PVDF+5% CoFe₂O₄ nanocomposites has no negative effect on cell viability. Alizarin red staining revealed that magnetic stimulation of PVDF+5% CoFe₂O₄ nanocomposites affects the processes of cell mineralization: in the groups with nanocomposites stimulation a greater number of large mineralization foci was observed compared to the control group and the group of cells cultured without magnetic stimulation of nanocomposites.

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Posters

Switching magnets setup FOR MAGNETO-MECHANICAL CELL DESTRUCTION

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Modern scienceis actively seeking new methods and technologies for the treatment of cancer. One of the promising methods in this field is magnetomechanical therapy, which uses low-frequency magnetic fields with strengths typically from 10 to 100 mT to guide and/or control magnetic nanoparticles to destroy cancer cells [1]. The shape and size of magnetic nanoparticles play an important role in their cancer treatment effectiveness. Anisotropic nanoparticles (e.g., nanodiscs or nanowires) can interact with cells more effectively and provide better tumor penetration due to enhanced permeability and retention effects, and their size can range from 1 to 1000 nm [2]. These nanoparticles can be made of different chemical elements such as iron oxides, nickel or ferrites and be capable of different kinds of motion such as rotational and/or translational. A minimum force of 1 to 100 pN is required to effectively rupture cell membranes, which depends on the characteristics of the nanoparticles, the magnitude of the magnetic field strength and its gradient [2]. Combination of magnetomechanical and photothermal therapies can increase the treatment effectiveness, but imposes additional restrictions on the temperature of the electromagnet to avoid damage to healthy tissues.

To study the magnetomechanical properties of nanoparticle solutions, we have developed an experimental setup consisting of a pair of switching dipole electromagnets. Its magnetic field and operational characteristics were studied. The parameters of the setup are as follows: operating frequency range $1\div100$ Hz, maximum pulsed current up to 7 A, voltage up to 100 V and magnetic field up to 75 mT. The working area is a 5 cm diameter circle with a gap between the magnets to accommodate a 96-well plate, standard for in vitro experiments. The unit can be operated continuously for 10 to 45 minutes with a maximum heating up to 44 degrees Celsius, with a purge system provided to protect the plate from heat. The unit also supports combination with photothermy by having an open optical axis along the axis of the electromagnets.

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The study of composite systems based on ferromagnetic microwires

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Multiferroic flexible polymer composites with nano- and micro-sized ferromagnetic active component (nano- and microparticles) are at the peak of popularity in studies devoted to the creation of technologies designed for energy collection and processing, as well as for biomedical applications - in terms of creating multiferroic scaffolds to accelerate the proliferation of neuronal cells [1-3]. Such composites are interesting from the point of view of applications, but issues related to the study of internal magnetic interactions of the filler and its effect on changing the multiferroic properties of the composite have not been fully studied.

This project is devoted to the development, creation and research of a new type of multiferroic composites with Fe-based ferromagnetic microwires for energy harvesting systems. The project is aimed at achieving not only a qualitative, but also a quantitative understanding of the process of converting small magnetic fields into electric ones through a comprehensive study of the correlation of this mechanism with the physical properties of ferromagnetic Fe-based microwires and the piezoactive matrix, as well as their interactions. For the first time, ferromagnetic microwires made of iron-based alloy (Fe) will be used as a magnetic component, having a positive magnetostriction coefficient, capable of rapid mechanical response to small changes in the external magnetic field [4,5], while piezoactive polymers will be used as a piezoactive matrix (biocompatible polyvinylidene fluoride (PVDF) capable of rapidly responding to mechanical microdeformations caused by the interaction of the ferromagnetic filler inside the matrix, as well as the magnetostrictive property of the filler.

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Improvement of Interfacial Interaction in the C₆₀/PVDF Nanocomposites by Trifluoromethylation

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The demand for two-phase composites is growing all over the world, since their combined properties - mechanical, thermophysical and technological - exceed those for single-phase materials. Carbon filler-based composites are known for their high strength, high temperature stability and excellent thermal conductivity. However, the problem in the technology of polymer composite materials with solid fillers is the incompatibility of phases due to weak adhesive interaction in the interfacial region. To solve this problem, fillers are often coated with organic compounds for better adhesion to the polymer matrix through hydrogen bonds. This strategy also makes it possible to achieve a better distribution of the filler over the volume of the polymer matrix [1]. A different approach based on the use of a modified filler to enhance intermolecular interaction is presented in this work. We explore the fabrication of two series of polyvinylidene fluoride (PVDF)-based composites with variable C_{60} and, for the first time, S_6 - $C_{60}(CF_3)_{12}$ concentrations (0.0, 0.3, 0.5 and 0.7 wt%) by the solution casting technique without stretching process and two similar series of stretched samples in the form of thin films with the thickness of $\sim 30 \, \mu m$. Our findings reveal that the presence of C₆₀ molecules provokes the formation of the β-phase of PVDF in unstretched films, while the content of the γ-phase decreases. The same, but even more pronounced trend is observed in stretched samples. Such changes in the phase composition are also recorded in the case of S_6 -C₆₀(CF₃)₁₂ molecules, however, the above dependence is greatly enhanced. These data correlate well with the conducted mathematical modeling, during which an increased interaction between PVDF and fullerenes during filler functionalization was established.

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The magnetic response and nucleation of fractal-like aggregates

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Magnetic nanoparticles can be taken up by cells, resulting in the formation of non-dense aggregates. These aggregates can be considered as multi-core particles (MCPs). The different spatial arrangements of the nanoparticles (granules) within the MCP result in a specific response to an applied magnetic field. In this study, several series of fractal-like MCPs with different numbers of magnetic granules and fractal dimensions are assembled. Idealized quasi-spherical MCPs with the arrangement of granules in the nodes of a simple cubic lattice were also considered.

The algorithm for MCP formation was based on the random attachment of granules to the central particle. Computer Monte Carlo simulations are used to predict the magnetic response of the constructed MCPs and to investigate the influence of the structure on the static magnetic properties of the MCP.

It was shown that the MCP magnetization is larger for aggregates with lower fractal dimension. This is due to the formation of compensating contours of magnetic moments of granules in MCP with large fractal dimension. It was observed that the arrangement of the granules in the MCP mainly in the field direction, promotes a more efficient alignment of magnetic moments, which increases the magnetic susceptibility and magnetisation of the MCPs. The formation of magnetic moments closed loops was studied by example of the quasi-spherical MCPs with magnetic granules located at the nodes of a cubic lattice as maximally packed structure. The magnetic moments of particles in close contact can strong interact with each other, creating complex magnetic configurations. Such closed loops can lead to a self-consistency effect, when internal interactions between magnetic moments become dominant compared to the effect of an external magnetic field. As a result, the MCP can demonstrate lower sensitivity to changes in the external field, which can be useful in applications where stability of magnetic properties is required.

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Magnetic and Magneto-Optical Properties of One-Dimensional Magnetoplasmonic Crystals with Broken Mirror Symmetry

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The use of nanomaterials is increasingly relevant and in high demand across various fields of science and technology. One specific type of nanomaterials is magnetoplasmonic crystals (MPlCs), which are nanostructures composed of metallic films deposited on diffraction gratings. In MPlCs, an enhancement of the Transversal Kerr effect (TKE) is observed due to the excitation of surface plasmon-polaritons (SPPs) [1]. These structures can be effectively utilized as concentration or magnetic field sensors [2, 3].

In this work, the samples were fabricated using oblique angle deposition magnetron sputtering using the ORION system, manufactured by AJA International. During the experiment, a 300 nm layer of permalloy (Ni₈₀Fe₂₀) was deposited at an angle of 85° onto silicon wafer substrates and polymer diffraction gratings with period of 740 nm and stripe's height of 100 nm.

The morphology of the fabricated samples was examined using an NT-MDT Spectra NTEGRA AURA atomic force microscope. The magnetic properties were analyzed with a LakeShore VSM7400 vibrating sample magnetometer. Optical and magneto-optical properties were studied using the handmade spectroscopy setup made of a halogen lamp, two GT-10 polarizers by Thorlabs, a pair of electromagnets, an OCV-6300 optomechanical modulator from Avesta, an MS-6400i monochromator by Sol Instruments, and a Thorlabs PMM01 photomultiplier tube with a SR830 Lock-In amplifier by Stanford Research Systems as a detecting system. Optical measurements were conducted in p-polarized light in a wavelength range from 600 to 900 nm at an incidence angle of 68°, in order to satisfy the SPPs excitation conditions at the -2 diffraction order. The samples were illuminated at various azimuthal angles relative to the plane of light incidence and the direction of the stripes on the substrate. At = 0°, the plane of light incidence was perpendicular to the tracks on the substrate.

The experiment showed that the spectral dependencies of the reflectivity demonstrate a pronounced dip at wavelengths of $\lambda=712\pm2$ nm and $\lambda=717\pm2$ nm at azimuthal angles of 0° and 180°. In the TKE spectra for the MPlCs , a slight enhancement was observed within the wavelength range corresponding to the reflectivity dip.

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The magnetic response of multi-core particles with different microstructures: the role of interparticle interactions

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The ability to control the magnetic properties of an ensemble of magnetic nanoparticles is of great interest in biomedical applications. In practice, a biological cell can absorb a limited number of magnetic particles, which, after entering, lose their ability to rotate and move, forming a single aggregate. The entire system forms a so-called multi-core particle. Moreover, different internal arrangements of granules and interparticle interactions can affect the magnetic response of the entire system. Let us consider a multi-core particle (MCP) consisting of granules arranged in the nodes of a simple cubic lattice. The length of the lattice edge is measured in units of the granule diameter and for close contact is one diameter. Different types of spatial structure of such MCPs are divided into two groups: with an even and an odd number of granules. In both cases, the positions of the granules in space are fixed.

The magnetic properties were studied using Monte Carlo computer simulation, during which attempts to change the orientation of the magnetic moment were made and the transition to the next configuration was carried out using the Metropolis algorithm. A uniform magnetic field was directed along the laboratory axis of the OZ and the total magnetic moment of the MCP in projection onto the axis and the initial magnetic susceptibility were calculated. In addition, to analyze the degree of ordering of magnetic moments in the absence of a field, a scalar order parameter S was used, taking values from 0 to 1, where the case of equality 1 means complete alignment of magnetic moments relative to the general direction and as the value decreases, the directions become "disordered".

It turned out that the magnetic moments of MCPs with an even number of granules, due to dipole-dipole interactions, tend to close into ring-shaped structures with close contact. The presence of such contours significantly complicates the magnetization of such MCPs in comparison with odd configurations. The effect of forming such structures disappears as the granules move away from each other. Among MCPs with an odd number of granules the MCP with turned out to be the most effective in terms of magnetic sensitivity, its magnetic moments immediately respond to the external field. At the same time, it is the MCP with 7 granules that is least susceptible to the formation of closed contours, since its susceptibility turns out to be little sensitive to the change in the interparticle distance and agrees well with the Langevin theory. An interesting effect of orientational texturing of magnetic moments is observed for the MCP with number of granules. Analysis of the fact of a monotonic decrease

in the parameter S in the absence of an external field indicates the formation of a special configuration of magnetic moments corresponding to a "chaotic" state, as opposed to the case of complete parallel alignment of the magnetic moments of the granules. Further study of the resulting orientational structures shows the emergence of nearly perpendicular pairs of magnetic moments, and as the intensity of the interparticle interactions increases, these pairs tend to unfold perpendicularly to each other.

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Investigating composite microdiscs as a potential agent for biomedical applications

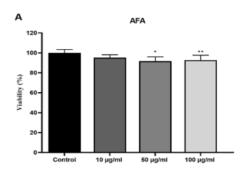
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Photothermal therapy (PTT) holds significant promise as a potential anti-cancer treatment due to low invasiveness and minimal side effects compared to traditional treatments such as chemotherapy, surgery, and radiotherapy. PTT most commonly utilizes noble metal nanoparticles that exhibit excellent photothermal properties. When laser irradiation is applied to tumor sites containing such particles, localized hyperthermia occurs. That exceeds the cell damage threshold, leading to the destruction of cellular structures and thermal cell death. In the context of complex diseases such as cancer, PTT is often selected as one component of a combination treatment strategy rather than as a stand-alone, all-purpose therapy. We propose PTT in combination with magnetomechanical therapy to achieve enhanced efficacy against cancer cells using gold-containing magnetic composite nanomaterials. Magnetomechanical therapy use a mechanical effect on the cell membrane by rotating magnetic nanoparticles in an alternating magnetic field of low frequency (about 1-10 Hz), which can trigger apoptotic processes in the cell exposed to magnetic nanoparticles. In comparison with spherical nanoparticles, microdisc-shaped particles have a higher mechanical moment and can be effectively used for magnetomechanical cell destruction in combination with PTT. In. this study microdisks consisting of gold and iron layers were manufactured as the studied architectures of magnetic nanocomposites using electron-beam lithography and magnetron sputtering.

The effect of gold-iron-gold microdiscs (AFA) and iron-gold-iron microdisks (FAF) on human hepatocarcinoma cells (Huh7) was studied before and after PTT and magnetomechanical therapy. Viability was assessed using the WST-1 test. The relative viability of Huh7 cells after 24 h of exposure with AFA shows slight significant decrease up to 8% (p < 0.0332) at 100 μ g/ml concentration, while FAF microdisks show a 11% (p < 0.0332) cytotoxic effect at a concentration of 100 μ g/ml. After PTT with microdisks of both compositions, the relative viability of the culture decreases. The temperature of the cell environment during PTT is on average from 43 to 45°C.



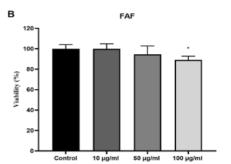


Figure 1. Viability of Huh7 cells after 24 h treatment with 10, 50 μ g/ml and 100 μ g/ml AFA (A) and FAF (B) microdiscs. Data normalized to values of control cells viability. Data statistical significance levels between treatment and control groups are represented by asterisks ("*" for p value < 0.0332, "**" for p value < 0.0021).

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Development of a high-precision mechanical stress mapping system

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Improper foot positioning during an incorrect walking/running leads to excessive strain on joints and other parts of the musculoskeletal system, resulting in foot pain, sprained tendons and excessive strain on certain bones and muscles. All this impairs the quality of life and, if the load is not distributed correctly over a long period of time, can also evolve into injuries and diseases that will cause discomfort in the long term. This is why a specialized high-precision mechanical stresses mapping system is required, which can read the pressure of the foot, thus avoiding the development of the described health problems.

Polyvinylidene fluoride (PVDF) is a polycrystalline polymer, in which one of the allotropic phases possesses a piezoelectric effect that allows a signal to be received when the pressure is applied. To enhance the piezoelectric signal, the new two-dimensional material from the family of MXenes can be used as a filler in the host PVDF matrix. MXenes are a new class of two-dimensional materials with the general formula Mn+1XnTx, where M is a transition metal, X is carbon and/or nitrogen, Tx is a functional group, and n is an integer index typically varying from 1 to 4. One of the MXenes' characteristic properties is their negatively charged surface. When they are placed into a polymer matrix, sets of nanocapacitors are being formed, which, when deformed, contribute to the amplification of the piezoelectric effect.

In this work, a polymer-based composite material PVDF-MX was created. A controlled push-pull setup was created to read out the piezoelectric response from this material when applying mechanical stresses. This setup allows the developed piezoelectric sensor to be calibrated. An electrical circuit was then designed to transmit data from the sensor to the PC via Bluethooth. Specialized software was developed for the PC (as well as for Android OS) to build 2D and 3D load distribution maps and to provide recommendations to improve foot placement. As a result of this work, a device consisting of 8 PVDF-MX piezoelectric sensors was successfully created, which can act as a tool to precisely map the distribution of mechanical stresses over the area of 5.2 per 1.3 cm. The developed device can be further used in orthopedy, professional sports or even on a mass market to analyze patterns of weight distribution over peoples' feet in static and dynamic regimes to prevent diseases and injuries related to the improper foot positioning.

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Measurement of the piezoelectric constant d33 of composite materials

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Modern challenges in the field of nature management and improving the efficiency of electrical equipment used in all areas of human activity require continuous improvement of energy-efficient design methods for systems. One approach to the solution is to use devices designed to collect noise electromagnetic energy generated by electrical devices [1,2]. The principle of constructing such systems is based on the transition of magnetic waves emitted by equipment into electrical energy, which can be achieved through transitions in multiferroic composites - materials that combine the properties of several ferroic phases, such as ferromagnetic (FM), ferroelectric and ferroelastic [3,4]. When using the direct magnetoelectric effect (ME) - energy transfer from the ferromagnetic phase to the ferroelectric, the application of an external magnetic field leads to a change in the macrosizes of the magnetostrictive component, which, due to the mechanical connection of the phases, leads to deformation of the piezoelectric component, thereby causing a change in the electric polarization in it. The issue of studying the mechanisms of improving piezoelectric properties and their control is acute.

This paper considers a variant of a self-assembling installation for measuring piezoelectric properties, in particular, the piezoelectric constant d33.

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Mechanical Properties of Fiber Composites with Climate- Regulating Properties

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This study presents the results of an analysis of the mechanical properties of fiber composites containing high-dispersion fillers based on phase change materials (PCM). These fillers possess a unique ability to absorb and release thermal energy during transitions between aggregate states, which opens new opportunities for application in various industries such as the textile industry, construction, automotive sector, and aerospace industry [1], [2].

Laboratory samples of fiber composites were produced using a melt mixing method in a twin-screw micro-extruder, followed by extrusion through a die with a diameter of 0.5 mm. The samples were then subjected to uniaxial orientation stretching at a rate of four times. The assessment of mechanical properties was conducted using the uniaxial tensile testing method, recording stress-strain diagrams. To investigate the climate-regulating effect in the composites, differential scanning calorimetry was employed. The surface structure of the samples was examined using a scanning electron microscope.

It was found that the addition of small concentrations of high-dispersion fillers leads to a 22% increase in tensile strength compared to filler-free samples. Thermal analysis revealed the temperature range of the phase transition for the endothermic process, which is found to be between 18 and 31 °C. The peak phase transition temperature occurs at 24 °C, with a transition energy of 3.58 J/g. The fiber composites exhibit a uniformly smooth surface, with diameters ranging from 200 to 250 micrometers.

The research demonstrated that the use of PCM enhances the deformation strength characteristics of fiber polymer composites, providing not only increased mechanical strength but also the creation of materials with climate-regulating effects. These studies highlight the potential for the application of fiber composites with PCM in the production of specialized technical textiles, including sporting goods, personal protective equipment, and medical devices.

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Magnetically Functionalized MXene Composites for Heavy Metal Sorption: Cu(II), Pb(II) and Fe(III)

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Two-dimensional MXenes ($Ti_3C_2T_x$) are a promising platform for heavy-metal adsorption due to their high specific surface area, hydrophilicity and negatively charged surface. However, their practical use is limited by the difficulty of separating the sorbent from aqueous solutions. Functionalization with magnetic Fe_3O_4 nanoparticles enables facile magnetic recovery without loss of sorption performance.

To perform a comparative kinetic analysis of the sorption of Cu(II), Pb(II) and Fe(III) ions from water using magnetically functionalized $Ti_3C_2T_x/Fe_3O_4$ composites, elucidating interaction mechanisms, kinetic parameters and thermodynamic characteristics.

Methods

- **Synthesis:** MXene via the MILD method, followed by co-precipitation of Fe₃O₄ nanoparticles at 80 °C.
- Characterization: XRD for phase identification; VSM showing saturation magnetization of $32 \pm 3 \text{ A} \cdot \text{m}^2/\text{kg}$ for the composite vs. $72 \pm 4 \text{ A} \cdot \text{m}^2/\text{kg}$ for pure Fe₃O₄;
- **Sorption Experiments:** Conducted at pH 5, sorbent concentration 10 mg/L, metal ion concentration 100 mg/L, temperatures 293–313 K.
- **Kinetic Models:** Pseudo-first order, pseudo-second order and intraparticle diffusion.

Results

- Cu(II) & Pb(II): Sorption follows pseudo-second-order kinetics (R²>0.99). Activation energies were -61.5 kJ/mol for Cu(II) and -24.8 kJ/mol for Pb(II), indicating a mixed chemisorption-diffusion mechanism for Cu and predominantly diffusion-controlled uptake for Pb. Intraparticle diffusion rates are an order of magnitude slower than external diffusion, likely due to the 2D MXene structure.
- **Fe(III):** Maximum capacity reached 9.36 mmol/g, with pseudo-second-order kinetics ($R^2 > 0.999$) and an activation energy of -17 kJ/mol, pointing to diffusion-limited sorption. Optimal pH range was 4–6, and equilibrium was achieved in ≈ 1 min.

Conclusion

Magnetic $Ti_3C_2T_x/Fe_3O_4$ composites demonstrate high efficiency and selectivity for removing Cu^{2^+} , Pb^{2^+} and Fe^{3^+} from aqueous solutions, combining capacities up to ~ 5.6 mmol/g (Pb at 313 K) with simple magnetic separation. The observed pseudo-second-order kinetics and diffusion limitations highlight the need to optimize sorbent structure to accelerate intraparticle transport of ions.

Acknowledgement:

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