Conference materials
UDC 539.192
DOI: https://doi.org/10.18721/JPM.183.255

Scattering of ultrashort laser pulses on some polymers and plasmids

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Abstract. The paper shows a method for the theoretical calculation of the spectrum of interaction between an ultrashort laser pulse and complex polyatomic objects. The calculation is shown on some plasmids DNA. The special feature of the calculation is the speed of processing the results. The method allows you to consider the scattering on all the atoms included in the molecules, while the calculation is performed quickly enough, due to the use of symmetries in the structure of the object in question. The method is suitable only for molecules with repeating regions in their structure, such as some plasmids and polymers, including DNA molecules with repeating nitrogenous bases. The calculation is based on the Hartree–Fock–Slater method. Before mathematical modeling, the molecule is built in the Avogadro program. The coordinates of the constructed model are used for the calculation. To date, the processing of experimental data obtained during operation of ultrashort pulses is difficult. The proposed method can help in deciphering the experimental data and reduce the processing time of the results.

Keywords: ultrashort laser pulses, plasmids DNA, scattering spectra

Funding: The research was supported by the state task of the Russian Federation No. FSRU-2024-0005.

Citation: Kharlamova A.A., Scattering of ultrashort laser pulses on some polymers and plasmids, St. Petersburg State Polytechnical University Journal. Physics and Mathematics. 18 (3.2) (2025) 275–279. DOI: https://doi.org/10.18721/JPM.183.255

Материалы конференции
УДК 539.192
DOI: https://doi.org/10.18721/JPM.183.255

Рассеяние ультракоротких лазерных импульсов на некоторых полимерах и плазмидах

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Аннотация. В статье представлен метод теоретического расчета спектра взаимодействия ультракороткого лазерного импульса со сложными многоатомными объектами. Расчет показан на примере некоторых плазмидных ДНК. Особенностью расчета является время обработки результатов. Метод позволяет учитывать рассеяние на всех атомах, входящих в состав молекул, при этом расчет выполняется достаточно быстро, благодаря использованию симметрий в структуре рассматриваемого объекта. Этот метод подходит только для молекул с повторяющимися участками в их структуре, таких как некоторые плазмиды и полимеры, включая молекулы ДНК с повторяющимися азотистыми основаниями. Расчет основан на методе Хартри–Фока–Слейтера. Перед математическим моделированием молекула строится в программе Avogadro. Для расчета используются координаты построенной модели. На сегодняшний день обработка

экспериментальных данных, полученных при работе с ультракороткими импульсами, затруднена. Предлагаемый метод может помочь в расшифровке экспериментальных данных и сократить время обработки результатов.

Ключевые слова: ультракороткие лазерные импульсы, плазмидная ДНК, спектры рассеяния

Финансирование: Исследование проводилось при поддержке государственного задания Российской Федерации № FSRU-2024-0005.

Ссылка при цитировании: Харламова А.А. Рассеяние ультракоротких лазерных импульсов на некоторых полимерах и плазмидах // Научно-технические ведомости СПбГПУ. Физико-математические науки. 2025. Т. 18. № 3.2. С. 275–279. DOI: https://doi.org/10.18721/JPM.183.255

Introduction

Currently spectroscopy is one of the most promising methods for studying complex molecular structures. There are different types of radiation used in spectroscopy, but in present, one of the most popular types is ultrashort laser pulse spectroscopy. With their help, many models of proteins and molecules have already been deciphered, as indicated by the marks in the world database of proteins and molecular compounds [1–3]. Using ultrashort pulses allows you to work on the same time scale as a molecule. Thus, it becomes possible to study the structure of a molecular compound before it changes, for example, under the influence of the environment. This is relevant specifically for protein compounds, since they are the ones that are difficult to crystallize, which complicates the experiment by other methods. To date, experiments using ultrashort pulses are actively underway in Hamburg, at a free electron laser installation. Decoding the received data is a complex process, especially if the object under study is a polyatomic structure. There are different ways to decipher the spectra obtained during scattering, but all of these are quite laborious and time-consuming. This article will show a method that reduces the calculation time for the model of the scattering spectrum of ultrashort laser pulses using examples of some plasmids and polymers.

Materials and methods

The calculation is based on the method described in [4, 5]. The method is derived from a theoretical description of the interaction of an ultrashort pulse with a test substance using numerical modeling and the Dirac–Hartree–Fock–Slater model. To simplify the decoding of molecular structures, it is proposed to conduct theoretical modeling of the interaction in order to obtain a reference diffraction pattern. But if there are repeating sections or links in the studied molecule, then the method can be simplified. The main calculation of the spectrum is carried out according to the formula:

$$\frac{d^2\varepsilon}{d\Omega_{\mathbf{k}}\, d\omega} = \frac{\left[\mathbf{E}_0\mathbf{n}\right]^2}{\left(2\pi\right)^2}\frac{\left|\tilde{h}\left(\omega\right)\right|^2}{c^3}\left\langle \sum_{i=1}^{s} N_{e,i}N_{A,i}\left(1-\left|F_i\right|^2\right)+\sum_{i,j=1}^{s}\delta_{i,j}N_{e,i}N_{e,j}F_iF_j^*\right\rangle, \qquad (1)$$

where $N_{e,i}$ is the number of electrons in the atom of the ith variety; $N_{A,i}$ is the number of atoms of the ith variety. $F_i = \frac{1}{N_{e,i}}\int \rho_{e,i}\left(\mathbf{r}\right)e^{-i\mathbf{pr}}d^3\mathbf{r} = 1$ is a form factor of the atom of the ith variety with an electron density $\rho_{e,i}(\mathbf{r})$.

Coefficient $\delta_{i,j} = \sum_{Ai,A'j} e^{-i\mathbf{p}\left(\mathbf{R}_{Ai}-\mathbf{R}_{A'j}\right)}$ depends only on the coordinates of atoms of the ith variety

(with *Ai* number), which position is determined by the radius vector $\mathbf{R}_{Ai}$. Eq. (1) is analytical, which contributes to a fairly simple calculation of spectra. The calculation of the electron density is difficult here. But if there are repeating sections in the molecule, the interference factor can be calculated in another way:

$$\delta_{i,j} = \sum_{\alpha=1}^{S} \sum_{n_\alpha=0}^{N_\alpha} e^{i\mathbf{p}\mathbf{R}_{n_\alpha}} \sum_{A_i \in R_{\alpha,1}} e^{i\mathbf{p}\mathbf{R}_{A_i}} \sum_{\beta=1}^{S} \sum_{n_\beta=0}^{N_\beta} e^{-i\mathbf{p}\mathbf{R}_{n_\beta}} \sum_{A_j \in R_{\beta,1}} e^{-i\mathbf{p}\mathbf{R}_{Aj}}. \quad (2)$$

Here, the interference factor is calculated by the sum of the repeated sections. For example, a DNA molecule has three repeating nitrogenous bases. Calculations within a single nitrogenous base are taken into account, and then the result is summed up by the number of repetitions. In this paper, the varieties of plasmids' ring forms are considered: one ring and two rings. Interestingly, gel electrophoresis is mainly used to study such structures. In the gel, plasmids begin to move under the influence of electricity, and the magnitude of their movement in the gel helps to distinguish large ring shapes from smaller ones. The ring plasmid of DNA is a closed DNA helix. Let us replace one spiral period with one element, as illustrated in Fig. 1.

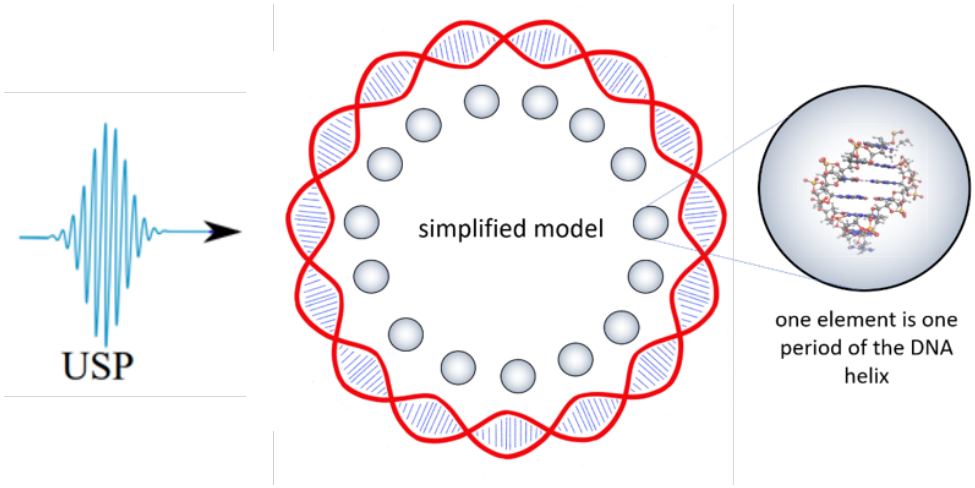

Fig. 1. Simplified model of the DNA ring plasmid

The position of plasmid DNA after gel electrophoresis in agarose gel provides an understanding of its structure. The method is simple and relatively inexpensive, and it has proven itself well. But this method couldn't help to evaluate changes in plasmids, such as ruptures. In addition, the method has a high error rate, since the difference between some forms of plasmids is small, for example, one ring and two rings of the DNA helix. In this paper, the use of ultrashort pulses for the analysis of such structures is proposed. Let us perform the calculation on the simplified structure of two ring plasmids. A supercoiled DNA plasmid will be used as the second sample for the study in Fig. 2.

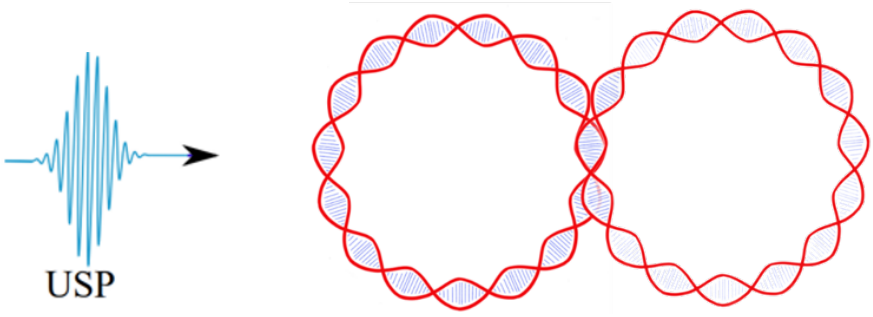

Fig. 2.Simplified model of a doubled circular DNA plasmid

Results and discussion

In this study the main objective is to identify the difference in the shapes of the spectra from two circular DNA plasmids. These shapes are interesting because despite a complex geometric arrangement of atoms in the structure, their number may practically not change. It is necessary to check whether the proposed method can capture changes only in the geometric position of the atoms. A simplified form of DNA plasmids, idealized rings, is used for this task. Theoretical modeling of the interaction of an ultrashort laser pulse with plasmids obtains results that shown on the following contour plots of scattering spectra (Fig. 3).

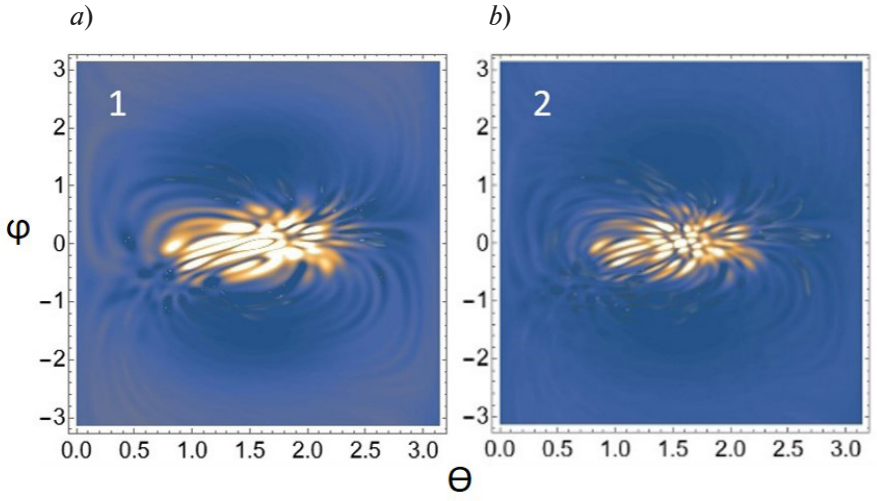

Fig. 3. Contour graph of the scattering spectrum during the interaction of an ultrashort laser pulse with a plasmid: ring plasmid of DNA (*a*); supercoiled plasmid of DNA (*b*)

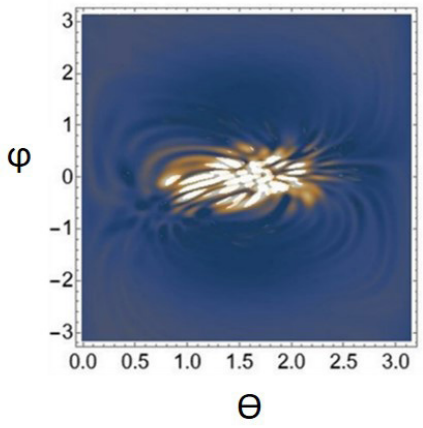

Fig. 4. Difference between the spectra. To visualize the difference between the obtained spectra, the contour graph images were superimposed on each other. The image of the DNA superplasmid spectrum is cut out in white

Here θ is the angle between the spiral axis and the scattering direction *n*, φ is the angle between the x-axis and the projection n on a plane perpendicular to the axis of the spiral. As can be seen from the graphs obtained, the spectrum of the DNA plasmid has a large number of spots. This is due to the large number of atoms, as well as the re-emission in repetitive areas. The laser pulse irradiated DNA as shown in Figs. 1, 2. The spectra differ significantly, although they are based on the same shape and the position of the main spots near the central maximum has the same direction.

Conclusion

As a result, a method is shown that makes it possible to calculate the structure of DNA plasmids using a simplified model. According to the results, the method enables to detect changes in the plasmid structure. Using the proposed method, it is possible to more accurately assess the structure of complex DNA.

Acknowledgments

The research was supported by the state task of the Russian Federation No. FSRU-2024-0005.

REFERENCES

1. **Neil M.C.,** Free electron X-ray lasers, Science. (4) (2010) 814–821.
2. **Tet I.,** Compact X-ray free-electron laser emitting in the sub-angstrom region, Nat. Photon. 6 (2012) 540–544.
3. **Chapman H.N.,** Femtosecond X-ray protein nanocrystallography, Nature. (470) (2011) 73–77.
4. **Makarov D.N., Kharlamova A.A.,** Scattering of Attosecond Laser Pulses on a DNA Molecule during Its Nicking and Bending, Int. J. Mol. Sci. (24) 2023.
5. **Kharlamova A.A.,** Calculation of the Interference Coefficient of the Polyatomic Molecular Structure of DNA, J of Biomedical Photonics and Eng. 9 (4) 2023.

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Received 05.09.2025. Approved after reviewing 25.09.2025. Accepted 26.09.2025.