Publ. Astron. Obs. Belgrade No. 102 (2022), 78 - 79 *Progress Report*

STUDY OF TWO DIMENSIONAL CRYSTALS BY RAINBOW SCATTERING EFFECT

M. HADŽIJOJIĆ and M. ĆOSIĆ

Laboratory of Physics, "Vinča" Institute of Nuclear Sciences
National Institute of the Republic of Serbia, University of Belgrade,
P. O. Box 522, 11001 Belgrade, Serbia

Abstract. In this report we present results of our theoretical study of 5 keV proton transmission through graphene. For these proton energies and considered fluences energy losses, irradiation induced defects of graphene and diffraction effects are negligible in this process. Proton trajectories were obtained by numerical solving of Newton's equations of motion, and subsequently used for construction of the proton angular yield. In the scattering angle plane we identified lines, along which the angular yield is very large. These lines correspond to singularities of the function that maps proton initial positions to the respective scattering angles. In analogy with meteorological rainbow, these lines are named – rainbow lines. It was found that rainbow pattern can be partitioned into outer and inner rainbow lines. The former are generated by trajectories of protons which scatter in the close vicinity of individual atoms, while the latter are formed by protons scattering within the graphene hexagon. Dependence of the rainbow pattern on the interaction potential was carefully investigated, revealing that inner rainbows can be useful for studying proton-graphene interaction potential. Change in the interaction potential, caused either by variation of the model parameters or by reorientation, induces regular change in the rainbow pattern and corresponding angular yield. These changes, also called metamorphoses, follow strict rules of the catastrophe theory. We conducted a thorough study of these metamorphoses, which led to development of the morphological method, relying solely on the shape of the rainbow pattern and not on the exact position of the rainbow lines or the particle count. Firstly, the closed form of the scattering law was derived using the momentum approximation. Then we used elements of the catastrophe theory to provide a local model of the rainbow pattern and the index theory of algebraic topology to describe the evolution of the rainbow pattern via bifurcations of the critical points of the reduced potential. We demonstrated that pre-images of the rainbows in the impact parameter plane are attracted and repelled by the nearest saddles and maxima of the reduced proton−graphene interaction potential. The ridge maxima of the angular distributions were investigated and related to the spectrum of the Jacobian matrix of the map generated by the scattering law. Observed evolution was summarized into five simple principles were introduced, allowing an experimentalist to sketch a qualitatively correct pre-image of the rainbow pattern in the impact parameter plane, as well as the distribution of the reduced potential critical points. Benefit of the introduced method is that it is based on the study of shape, making it insensitive to noise.

Established morphological method was used for study of thermal vibrations and point defects of graphene. Thermal motion of atoms was incorporated by averaging the static proton-graphene interaction potential over the distribution of atom displacements. The covariance matrix of atom displacements was modeled by Debye theory, and calculated using Molecular Dynamics approach. It was shown that outer rainbow lines can be modeled by ellipses whose parameters are very sensitive to the structure of the covariance matrix. Numerical procedure was developed for extraction of the covariance matrix from the corresponding outer rainbow lines in the general case, when atoms perform fully anisotropic and correlated motion. We have studied transmission of protons through the graphene containing point defects. It was shown that each defect type produces its distinctive inner rainbow pattern. Finally, it was demonstrated how the acquired knowledge about inner rainbow patterns could be used to determine the unknown defect densities of the different defect types present in the same sample.The outer rainbow pattern caries information about the composition of the sample, while the inner rainbows informs about its structure. Therefore, these lines could be named compositional and structural rainbows, respectively. Moreover, we have shown that compositional and structural rainbows do not interact, making morphological analysis appropriate for characterization of the graphene-like materials.

References

M. Ćosić, S. Petrović, N. Nešković, The forward rainbow scattering of low energy protons by a graphene sheet, *Nucl. Instrum. Methods Phys. Res., Sect. B* **422**, 54 (2018)

M. Ćosić, M. Hadžijojić, S. Petrović, R. Rymzhanov, S. Bellucci, Investigation of the graphene thermal motion by rainbow Scattering, *Carbon* **145**, 161 (2019)

M. Ćosić, M. Hadžijojić, S. Petrović, R. Rymzhanov, The morphological analysis of rainbow scattering in graphene, *Chaos* **31,** 093115 (2021)

M. Hadžijojić, M. Ćosić, R. Rymzhanov, Morphological Analysis of the Rainbow Patterns Created by Point Defects of Graphene, *J. Phys. Chem. C*. 125, **38**, 21030–21043 (2021)