Giant planets offer help in faster research on material surfaces

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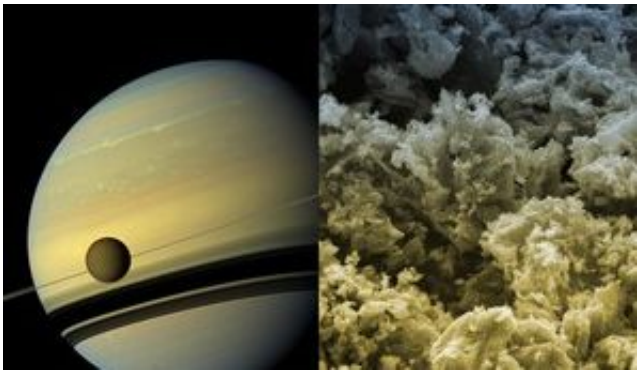

The modelling of phenomena observed in spectroscopic studies of material surfaces employs function discovered by S. Chandrasekhar in analysing interaction of light with atmospheres of giant planets. New algorithm for calculating the values of the function, much more accurate and a few dozen times faster than the existing algorithms, has been developed at the Institute of Physical Chemistry of the Polish Academy of Sciences in Warsaw. Left image: Saturn, the second largest gas giant in Solar System, and its moon Titan, from NASA's Cassini spacecraft. Right image: Surface of activated charcoal NORIT as seen by the scanning electron microscope FEI Nova NanoSEM 450 (mag. 5000x, false colours). Credit: NASA/JPL-Caltech/Space Science Institute, IPC PAS

New, fast and accurate algorithm from the Institute of Physical Chemistry of the Polish Academy of Sciences in Warsaw, based on the mathematical formalism used to model processes accompanying interaction of light with gas planet atmospheres, is a major step towards

better understanding of physical and chemical properties of materials' surfaces studied under laboratory conditions.

Solar System's gas giants, Jupiter and Saturn, are among the brightest objects in the night sky. We see them, because light from our star interacts with their dense atmospheres. The mathematical formalism describing the interaction of light with planetary atmospheres was developed in 1950 by Subramanyan Chandrasekhar, a famous Indian astrophysicist and mathematician. His two hundred pages long derivation involves a complicated function that more recently has been used, i.a., in studies on physical and chemical properties of material surfaces. Calculation of very accurate values of Chandrasekhar function still presents a challenge. The researchers from the Institute of Physical Chemistry of the Polish Academy of Sciences (IPC PAS) in Warsaw managed to develop a method for calculating the function with the accuracy of up to over a dozen decimal digits. The new algorithm combines different numerical methods and is much faster than the existing approaches.

Light entering a gas planet atmosphere is scattered via different mechanisms (elastically and inelastically). In addition, light waves of certain wavelengths are selectively absorbed by elements and chemical compounds contained in the atmosphere. "Usually, we believe that the star light is simply reflected from a planet as from a mirror. It is not true. The planet's atmosphere is a place where many phenomena related to radiation transfer take places", says Prof. Aleksander Jabłoński from the IPC PAS.

It turns out that physical models describing interaction of light with the gas giant atmosphere can also be used to describe emission of electrons following irradiation of material samples with x-ray beam. Photoelectrons of specific energy, leaving the surface of the sample, are emitted from a few atomic layers only. The electrons emitted at larger

depths loose their energies due to interactions with atoms of a solid. Analysis of photoelectron energies and intensities allows for assessing the properties of tested material.

"Using surface sensitive spectroscopic methods we are able to determine properties of the most external layers of materials, as well as their chemical composition or condition. This knowledge is of crucial importance in materials engineering, microelectronics, various nanotechnologies, and in so important processes as catalysis or ubiquitous corrosion", explains Prof. Jabłoński.

For years Prof. Jabłoński has been developing databases for the US National Institute of Standards and Technology (NIST). These databases contain certain parameters required in calculations needed for applications of electron spectroscopies to analyse properties of surfaces. One of such databases was entirely developed using the mathematical formalism close to that originally proposed by Chandrasekhar for the description of astronomical phenomena.

The calculations needed for processing of results of spectroscopic studies require multiple determinations of Chandrasekhar function values with the highest possible accuracy. Though the Chandrasekhar function describes a relatively simple physical phenomenon, it is a complicated mathematical expression. There are many methods for determining Chandrasekhar function values with a reasonably good accuracy, close to 1-2%. Some applications related to electron transport in superficial layers of materials require, however, that Chandrasekhar function is determined with a precision of more than 10 decimal digits.

"In recent years, I have been able to develop an algorithm that allows for obtaining such a high accuracy, and is up to a few dozen times faster in operation when compared with the existing algorithms", says Prof. Jabłoński. The increase in speed of algorithm operation is as important

as the increase in accuracy. This is due to the fact that in programs for modelling electron transport on surfaces of materials the Chandrasekhar function must be computed thousands, and even tens of thousands times.

The program code with implemented new algorithm for calculating Chandrasekhar function values was published in the *Computer Physics Communications* journal.

It is to be noted that Chandrasekhar function plays an important role not only in astronomy and physical chemistry of surfaces. The function has also found application in the nuclear power industry where it is used, i.a., for analysing electron scattering in nuclear reactor shields.

Provided by Polish Academy of Sciences

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