

Cracow, 8 November 2023

Cheap and efficient ethanol catalyst from laser-melted nanoparticles

Ethanol fuel cells are regarded as promising sources of green electricity. However, expensive platinum catalysts are used in their production. Research on laser melting of suspensions, carried out at the Institute of Nuclear Physics of the Polish Academy of Sciences in Cracow, has led researchers to materials that catalyse ethanol with a similar – and potentially even greater – efficiency to platinum, yet are made of an element that is many times cheaper than platinum.

When a suspension of nanoparticles is irradiated by laser pulses, the particles in the suspension can begin to melt and stick together permanently, while rapidly undergoing chemical reactions that are more or less complex. One of the recent materials obtained in this way, produced at the Institute of Nuclear Physics of the Polish Academy of Sciences (IFJ PAN) in Cracow, turns out to have an unexpectedly high efficiency in catalysing ethanol, a compound considered to be a promising energy source for fuel cells.

Ethanol is a fuel with many advantages – it can be produced in a renewable manner (for example, from biomass), it can be easily stored as well as having low toxicity. What is of particular importance, however, is the fact that up to several times the amount of electricity can be obtained from a unit mass of ethanol compared to current popular power sources.

Electricity in ethanol-powered fuel cells is generated by processes associated with the oxidation of this alcohol on the catalyst layer of the reaction. Unfortunately, current catalysts do not allow the rapid and complete oxidation of ethanol to water and carbon dioxide. As a result, the cells not only fail to reach maximum efficiency, but also produce undesirable by-products that are deposited on the catalyst and, over time, lead to the disappearance of its properties.

"A considerable obstacle to the commercial success of ethanol cells is also their price. The catalyst we have found can have a significant impact on its reduction and, consequently, on the availability of new cells on the consumer market. This is because its main component is not platinum, but copper, which is almost 250 times cheaper than platinum," says Dr. Mohammad Shakeri (IFJ PAN), first author of the paper in the journal Advanced Functional Materials.

The achievement of scientists from the IFJ PAN is the result of research conducted on laser control of the size and chemical composition of agglomerates in suspensions. The main idea behind the laser nanosynthesis of composites is the irradiation of a suspension containing agglomerates of nanoparticles of a specific chemical substance with pulses of unfocused laser light with appropriately selected parameters. The aptly delivered energy causes the temperature of the particles to increase, they melt on the surface and clump together into larger and larger structures, which cool rapidly on contact with the surrounding cool liquid. The temperature reached by the particles is determined by many factors, including the energy of the photons emitted by the laser, the intensity of the beam, the frequency and length of the pulses, and even the size of the agglomerates in suspension.

"Depending on the temperature reached by the agglomerates, various chemical reactions may take place in the material in addition to changes of a purely structural nature. In our research, we focused on the most accurate theoretical and experimental analysis of the physical and chemical phenomena in suspensions in which pulses of laser light were absorbed by nanoparticles of copper and its oxides," explains Dr. Zaneta Swiatkowska-Warkocka (IFJ PAN).

In the case of real solution particles, the temperature rise occurs in nanoseconds, too rapidly to be measured. In this situation, theoretical molecular dynamics analyses became the first step in understanding the copper systems under study, supported at later stages by simulations performed by the Prometheus computer cluster from Cracow. Thanks to these, the researchers determined to what temperatures the agglomerates of various sizes would heat up and what compounds might form in these processes. In addition, they checked whether these compounds would be thermodynamically stable or undergo further transformations. The physicists used the knowledge gained to prepare a series of experiments in which nanoparticles of copper and its oxides were laser fused in various proportions.

The composite materials obtained were tested in the laboratories of the IFJ PAN and in the Cracow SOLARIS cyclotron, among others, to determine the degree of oxidation of copper compounds. The information obtained allowed the researchers to identify the optimum catalyst. This turned out to be a three-component system built from appropriate proportions of copper and its oxides of the first and second oxidation state (i.e. Cu_2O and CuO).

"From the point of view of efficiency of ethanol catalysis, the crucial discovery was that particles of copper oxide Cu_2O_3 , which is usually thermodynamically very unstable, were present in our material. On one hand, they are characterised by an extremely high degree of oxidation, on the other hand, we found them mainly on the surface of the Cu_2O particles, which in practice means that they had very good contact with the solution. It is these Cu_2O_3 particles that facilitate the adsorption of the alcohol molecules and the breaking of the carbon-hydrogen bonds in them," states Dr. Shakeri.

Tests on the properties of the catalyst produced by the Cracow physicists ended with optimistic results. The selected composite retained the ability to fully oxidise ethanol even after several hours of use. Moreover, its electrocatalytic efficiency proved comparable to that of contemporary platinum catalysts. From a scientific perspective, this result is positively astonishing. Catalysis generally proceeds more efficiently the larger the surface area of the agglomerates, which has to do with the fragmentation of their structure. However, the composite studied was not nanometre in size, but several orders of magnitude larger, submicron in size. It seems likely, therefore, that if physicists succeed in reducing the size of the particles in the future, the efficiency of the new catalyst could increase still further.

The work on laser fusion of copper nanostructures was funded by the Polish National Science Centre.

The Henryk Niewodniczański Institute of Nuclear Physics (IFJ PAN) is currently one of the largest research institutes of the Polish Academy of Sciences. A wide range of research carried out at IFJ PAN covers basic and applied studies, from particle physics and astrophysics, through hadron physics, high-, medium-, and low-energy nuclear physics, condensed matter physics (including materials engineering), to various applications of nuclear physics in interdisciplinary research, covering medical physics, dosimetry, radiation and environmental biology, environmental protection, and other related disciplines. The average yearly publication output of IFJ PAN includes over 600 scientific papers in high-impact international journals. Each year the Institute hosts about 20 international and national scientific conferences. One of the most important facilities of the Institute is the Cyclotron Centre Bronowice (CCB), which is an infrastructure unique in Central Europe, serving as a clinical and research centre in the field of medical and nuclear physics. In addition, IFJ PAN runs four accredited research and measurement laboratories. IFJ PAN is a member of the Marian Smoluchowski Kraków Research Consortium: "Matter-Energy-Future", which in the years 2012-2017 enjoyed the status of the Leading National Research Centre (KNOW) in physics. In 2017, the European Commission granted the Institute has been classified into the A+ category (the highest scientific category in Poland) in the field of physical sciences.

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SCIENTIFIC PUBLICATIONS:

 "Alternative Local Melting-Solidification of Suspended Nanoparticles for Heterostructure Formation Enabled by Pulsed Laser Irradiation"
M. S. Shakeri, Ż. Świątkowska-Warkocka, O. Polit, T. Itina, A. Maximenko, J. Depciuch, J. Gurgul, M. Mitura-Nowak, M. Perzanowski, A. Dziedzic, J. Nęcki

Advanced Functional Materials, 33, 43, 2023 DOI: <u>10.1002/adfm.202304359</u>

LINKS:

http://www.ifj.edu.pl/ The website of the Institute of Nuclear Physics, Polish Academy of Sciences.

http://press.ifj.edu.pl/

Press releases of the Institute of Nuclear Physics, Polish Academy of Sciences.

IMAGES:

IFJ231108b_fot01s.jpg HR: <u>http://press.ifj.edu.pl/news/2023/11/08/IFJ231108b_fot01.jpg</u> Successive phases of agglomeration of nanoparticles of copper and its oxides, occurring in the first 200 picoseconds of laser melting: top in microscopic images (mag. 5000x), bottom in computer simulation. (Source: IFJ PAN)

MOVIES:

Simulation of laser melting of nanoparticles <u>https://www.youtube.com/watch?v=pcUKtqFpLqM</u> Simulation of laser melting of nanoparticles made of copper and its oxides. (Source: IFJ PAN)