Iron-aluminium compound could replace palladium catalyst, reducing the cost of plastic production

June 20 2012

An alternative to precious metal: Max Planck scientists used this crystal of an iron-aluminium compound to catalyse an important step in the production of polyethylene plastic. To date, industry has used a palladium compound for this process. © MPI for Chemical Physics of Solids

(Phys.org) -- Chemists don't like precious metals – at least not when they need the expensive materials as catalysts to accelerate reactions or guide them in a particular direction. And this is often the case, as in an important step in the production of polyethylene, a substance that makes plastic bags light, flexible and stable. However, a team of scientists from the Max Planck Institute for Chemical Physics of Solids in Dresden and the Fritz Haber Institute of the Max Planck Society in Berlin have now developed a catalyst using iron and aluminium that works just as well as the conventional palladium catalyst, but costs much less. To identify the iron-aluminium alternative, the scientists first systematically ascertained what properties the material would need. They plan to use this same procedure to search for catalysts for other reactions in future.

Were it not for the fact that the chemical industry routinely uses palladium as a reagent for polyethylene, plastic bags would be a great nuisance, ripping when loaded with just a couple of apples and a carton of milk. However, we are spared this fate by the reliable work of the precious metal. Palladium converts ethine, more commonly known as acetylene, into ethene, also known as ethylene, which is used to make polyethylene. Ethylene always contains traces of acetylene, because both substances are obtained from crude oil and are not easily separated. However, acetylene interferes in the conversion of ethylene to polyethylene. Thererforе, unless it is first converted to ethylene by the attachment of two hydrogen atoms in the presence of palladium, the resulting plastic is of poor quality.

Worldwide production of polyethylene amounts to 80 million tonnes each year, thus the costs of acetylene conversion add up to a considerable sum. However, these costs could drop significantly, as it may now be possible for industry to manage without the palladium catalyst, using an intermetallic compound of iron and aluminium instead. Working with the Ludwig Maximilians Universität Munich and Forschungszentrum Jülich, scientists from Dresden's Max Planck Institute for Chemical Physics of Solids and the Fritz Haber Institute of the Max Planck Society in Berlin have identified this material as an effective substitute for palladium, finding that it hydrogenates acetylene to ethylene just as efficiently as precious-metal catalysts.

The catalytically-active material must be present at tiny, isolated sites

"It was not by trial and error that we discovered that this compound is so suitable, but by a knowledge-based approach", says Marc Armbrüster of the Dresden-based Max Planck Institute. Knowledge-based means that the scientists used their knowledge of precisely how the reaction at the palladium catalyst occurs. They then deduced the critical aspects and searched for a suitable material with these criteria in mind.

Their first lead was the well-known fact that even palladium only delivers the desired results when it is present at the smallest possible active sites, e.g. as individual palladium atoms on an inactive silver matrix; otherwise the acetylene reaction does not stop at semi-hydrogenation. In this case, acetylene takes not two, but four hydrogen atoms and is converted to ethane, which is quite unsuitable for the chain reaction leading to polyethylene. "It seems that the acetylene molecules attach themselves to the tiny palladium sites in such a way that they can only selectively take up two hydrogen atoms", explains Marc Armbrüster. However, finely distributed palladium in a silver alloy gradually clumps into larger aggregates under the reaction conditions, and its selectivity becomes increasingly compromised.

Active sites can be kept strictly separate in an intermetallic compound

As they discussed this in 2004, Juri Grin, Director at the Max Planck Institute for Chemical Physics of Solids, and Robert Schlögl, Director at the Fritz Haber Institute of the Max Planck Society in Berlin, came up with the idea of fixing the active sites, i.e. the individual palladium atoms, in a crystal lattice. As a result, the following years saw them pool the core competencies of two Max Planck Institutes – for catalysis in Berlin and for intermetallic compounds in Dresden – to solve an important practical problem. This cooperation yielded immediate results, as the search for a suitable catalyst for the semi-hydrogenation of acetylene quickly revealed a gallium-palladium compound as the material of choice.

The fact that this is an intermetallic compound and not an alloy is decisive, partly because the metals do not mix haphazardly (as alloys do), but form highly ordered crystal structures. As a result, the atomic structure of an intermetallic compound differs from that of its components in their pure forms. In the case of the palladium-gallium compound, every palladium atom in the crystal structure is surrounded exclusively by catalytically inactive gallium atoms. This means that the individual catalytic sites are kept strictly separate from each other.

The palladium catalyst substitute must have a similar structure

The success of the basic idea encouraged the scientists to take the next step and search for a material that would exhibit catalytic properties like those of the palladium-gallium compound, but without the palladium. It was the crystal structure of the Al13Fe4 compound that caught their attention, as its aluminium atoms keep the iron atoms apart in exactly the same way that the gallium atoms separate the palladium atoms in the palladium-gallium catalyst.

However, this alone would not be enough to ensure a workable catalyst for acetylene conversion; the candidate compound would only be suitable if it converted acetylene molecules in the same way as the palladium catalyst. This question in turn depends largely on the distribution of electrons in the material, their energy and how they influence the binding of acetylene molecules. The aluminium-iron and palladium-gallium compounds are similar to one another in these aspects, and the iron-aluminium compound actually does deliver precisely two hydrogen atoms to the acetylene molecules just as reliably as the palladium-gallium catalyst.

The iron-aluminium catalyst could reduce production costs for many plastics

Before the new catalyst can be used to reduce the costs of polyethylene production, it must prove itself in industrial scale applications. If it passes that test, it could prove its value as a selective hydrogen catalyst in the production of other synthetic materials.

Meanwhile, the Dresden- and Berlin-based chemists want to systematically search for catalysts for other reactions. One important finding of their work is that the knowledge-based approach can spell success in catalysis research, and perhaps one day mean that the chemical industry can manage without any precious metals in its reactors. Many everyday products could then be cheaper – and that would be good news for more than just chemists.

More information: Marc Armbrüster, Kirill Kovnir, Matthias Friedrich, Detre Teschner, Gregor Wowsnick, Michael Hahne, Peter Gille, Lászlo Szentmiklósi, Michael Feuerbacher, Marc Heggen, Frank Girgsdies, Dirk Rosenthal, Robert Schlögl and Yuri Grin, Al13Fe4 as a low-cost alternative for palladium in heterogeneous hydrogenation, *Nature Materials*, 10 June 2012; doi:10.1038/nmat3347

Provided by Max Planck Society