A new theory to explain the transparency of metallic oxides

- The electrons of some metal oxides, due to their large effective mass when coupled with the ionic lattice of the material, cannot follow the electric field of light and allow it to pass through the material.
- Transparent and conductive materials are used in smartphone touch screens and solar panels for photovoltaic energy.

Researchers from ICMAB-CSIC have led a new theory to explain the transparency of some metal oxides, which proposes that the effective mass of electrons is large in this type of materials due to the formation of "polarons" or couplings between electrons in motion and the ionic lattice of the material, which is distorted around them. Electrons with this larger effective mass cannot rapidly oscillate following the electric field of light, and they let it pass rather than reflect it. The accepted theory so far was explained by the interactions between the electrons themselves.

Materials suitable for touch screens: transparent and conductive

Have you ever thought of what the touch screens of smartphones and ipads are made of? They are clearly made of a transparent material, but it is not glass, because glass would not be responsive to our fingers, since it is not conductive. The screens must be made of a transparent and conductive material. Most are made of a semiconductor material called "indium tin oxide," abbreviated ITO. Other applications of this material are solar panels, LEDs in liquid screen displays, LCD or OLED, and even in coatings of aircraft windshields.

It is quite a unique material, since in general it is difficult to find conductive materials that are transparent. Despite the many advantages it offers, it has a rather serious problem, which is that indium is a very rare metal. In fact, with the high production of touch screens and the expansion of photovoltaics, it is estimated that it will surely be finished up before 2050. Furthermore, it is the most expensive component of any mobile phone or tablet: the touch screen represents approximately 50 % of the cost of the device. This is why it is so important the research for potential new substitutes.

Heavy electrons cannot follow light and let it pass

In general, materials are transparent to visible light when photons of light cannot be absorbed by the material and pass through it without their journey being interrupted by interactions with electrons. This happens when there are no proper electronic transitions between the ground states and the excited states of the electrons. This is what happens in insulating materials, which have an energy band gap greater than the energy of photons, with which they cannot make them jump from one state to another, and there is no movement of charges. Window glass would be an example of a transparent and insulating material.

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The presence of free charges (electrons) is a fundamental characteristic in metals, which are conductors by nature. In these materials, the electrons, under the influence of the electric field of light, are forced to oscillate, and they radiate light at the same frequency as the receive light. This means that metals tend to shine, because they reflect the light that reaches them. In addition, this makes them opaque, since light does not pass through them. This explains how mirrors are made, formed by a thin metallic layer (behind a protective layer of transparent glass), which reflects all the light that reaches it. And it also explains why steel, aluminum, silver or platinum, for example, are colorless and very bright.

How fast electrons oscillate and the light they reflect depends on their mass. Free electrons are very light, therefore very responsive in the electric field of light, and will reflect light as we have explained. Now, the "heavier" electrons cannot follow the oscillations caused by the electric field of light so quickly, and cannot reflect it, but rather let it pass without interacting; the material is then transparent.

Looking for a substitute for ITO

But how can we get "heavy" electrons? How can we get a metal that is transparent?

ITO is a material synthesized from indium oxide, an insulating material with a large energy band gap, and transparent. It is made conductive and therefore suitable for touch screens, because the material is doped with tin atoms, which take up places on the indium atoms, and endow it with additional electrons. These free electrons are responsible for the material being conductive. There is an optimal point where the material is transparent and conductive, but if this point is passed, the material becomes more conductive, but acquires the reflection property of metals, and ceases to be transparent. This optimal point has already been well studied and there is no room for improvement in this regard.

The material that researchers from the Institute of Materials Science of Barcelona (ICMAB, CSIC) have studied, thinking that it could be a good substitute for ITO, is a vanadium and strontium oxide. It is a metallic material, but thin layers of this material have been surprisingly found to be transparent. Following the logic above, to be transparent, the mass of the free electrons would have to be large. How is that possible?

Polarons and the new theory explaining the transparency of the metal oxides

The currently accepted scenario to explain the transparency of this and other metallic oxides is that the electrons experience very strong electrostatic interactions between them, and they can no longer be considered independent particles, but are part of a set called “correlated electronic system”, which makes the effective mass of the electrons larger.

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Now, this new study, published in *Advanced Science* and led by researchers from ICMAB, proposes a totally different point of view. "We think that increasing the effective mass of electrons is due to their interactions with the lattice. The electrons of strontium and vanadium oxide and, in general, of metal oxides, move in a matrix of ions (positive and negative). This lattice is deformed by the moving electrons, and this distortion moves with it. It would be like an electron dressed with a distortion of the lattice moving through the material. This coupling between the electron and the lattice is called "polaron", and it is heavier than the free electron, so the effective mass of the electron is greater, which would explain the transparency of the material to visible light, since it cannot follow the oscillations of the electric field of light, and let it pass", explains Josep Fontcuberta, ICMAB researcher and leader of this study.

With this new theory, the paradigm established so far in the field of condensed matter physics is broken. Until now, it was accepted that coulombic interactions between electrons governed the properties of metal oxides. This new theory proposes instead that the interaction between electrons and the ion network plays a crucial role. And what it is more important: many of the experiments validate it.

A study from another point of view

The study contains a very complete and unprecedented analysis of some of the electrical and optical properties that are perfectly described with the "polarons" scenario. "In previous studies it had been seen that there could be a relationship, but it had never been analyzed in depth. Furthermore, apart from verifying the theory in tin and vanadium oxide, it has been analyzed in other metallic oxides and in some doped insulators, and it has been verified that the predictions are fulfilled", explains Fontcuberta.

"This study, among other things, is the result of a very exhaustive characterization of the electrical and optical properties of dozens of thin layers of the material in question. It is also the result of a very careful analysis of the data, which has revealed some discrepancies with scenarios and theories established long ago. The patient and meticulous work of Mathieu Mirjolet, ICMAB predoctoral researcher, has made this possible. I do not know if it has been the most relevant discovery of my career, since I do not know what is still to come, but I can assure you that it is one that best ways to illustrate my genuine pleasure in looking at science and life from another point of view" adds Fontcuberta.

The study has been led by ICMAB researchers from the MULFOX group, Josep Fontcuberta and Mathieu Mirjolet, where the materials have been synthesized and most of the characterization and analysis of the data has been carried out, in collaboration with researchers from the University of Santiago de Compostela (F. Rivadulla) and the University of Freiburg (P. Marisk), which have provided complementary measurements of the effective mass of electrons, and with the University of Frankfurt (R. Valentí), which has collaborated in the analysis of the properties of the polaron and of the thin layers of strontium oxide and vanadium.

Reference article:

Electron - Phonon Coupling and Elec tron - Phonon Scattering in SrVO3
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