METAL-INSULATOR TRANSITION

# The Mott transition in the light of synchrotron radiation

The Mott transition reflects the transition between the insulating state of a system of correlated electrons and a metallic phase (see box). Understanding this metal-insulator transition is essential, not only from a fundamental point of view but also to control the electronic properties of materials, with major technological implications in the search for faster and more efficient electronic devices.

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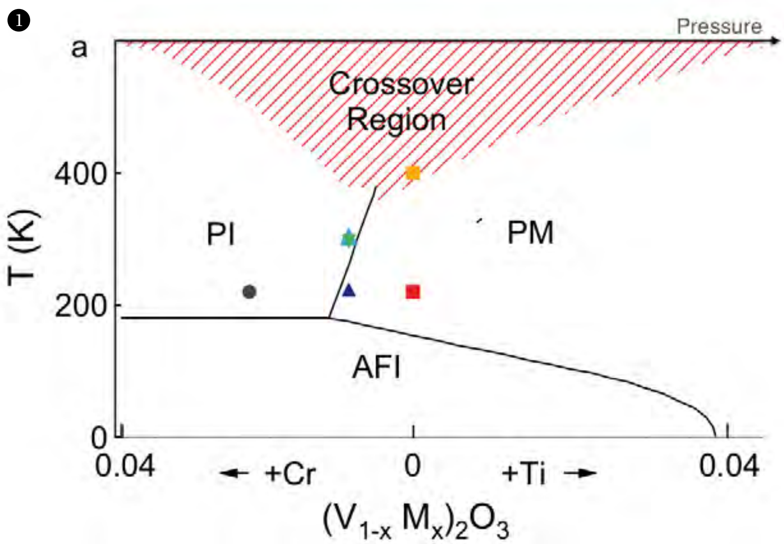


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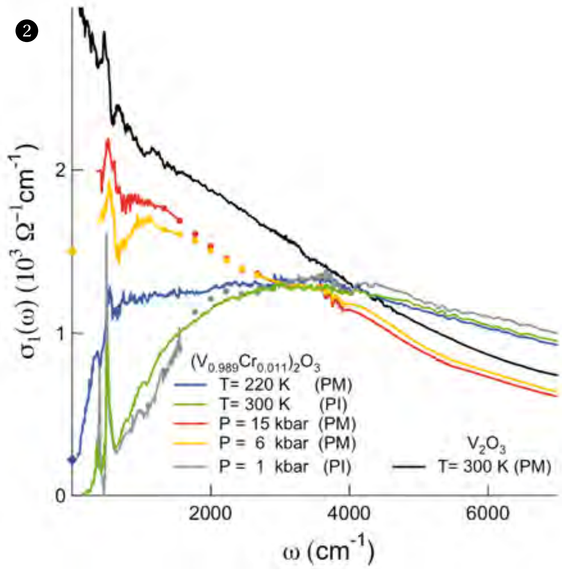


The Mott transition remains poorly understood and highly complex: the material has an intermediate behavior between metal and insulator that is poorly described by theory and difficult to characterize experimentally. The most advanced spectroscopic techniques using synchrotron radiation can provide answers to these open questions. As part of an international collaboration involving the University of Rome "La Sapienza" and the Laboratoire de Physique des Solides (LPS) at Orsay, researchers on the GALAXIES, PSICHE and CRISTAL beamlines, at SOLEIL undertook a study of the metal-insulator transition in Cr-doped $V_2O_3$, a model material of strongly correlated electron systems, using different techniques from infrared to X-rays. This work, which started as part of a SOLEIL/LPS PhD. thesis [1,2] has recently led to spectacular results obtained through an original approach combining electronic and structural probes.

## Not as simple as it seems

The phase diagram of $V_2O_3$ was established in the 1970's as a function of temperature, doping and pressure (Figure 1). Based on this diagram, $V_2O_3$ is metallic at room temperature (Paramagnetic Metallic phase, PM) and becomes insulating at low temperatures (Antiferromagnetic Insulating phase, AFI) or by doping with Cr (Paramagnetic Insulating phase, PI); in the latter case, it is possible to restore the metallic phase by applying external pressure (upper scale) from a doped sample or through temperature and appropriate doping (triangles). We focused more specifically on the PM-PI transition in $V_2O_3$-1.1% Cr doped compound. Unlike the PM-AFI transition, the PM-PI transition occurs without structural change and as such is considered as a pure manifestation of electron correlations and thus of the Mott transition. It soon became clear, however, that the apparent simplicity of the phase diagram masked great physical complexity: the behavior in the PM phase is that of a poor metal, the structure of $V_2O_3$-1.1% Cr has a mixture of phases; doping induces local distortions in the structure; finally, the transition mechanism remains poorly understood.

A first confirmation of this complexity came from measurements of optical conductivity in the infrared (Figure 2) obtained at ELETTRA. Although the PI phase clearly shows an energy gap - this is the signature of an insulator - (green curve), the spectra obtained in the metallic phase is highly sensitive to

**Figure 1: Phase diagram of $V_2O_3$ as a function of temperature (left scale), doping (below) and pressure (above). PI, PM are insulating and metallic paramagnetic phases, respectively, and AFI, the insulating antiferromagnetic phase.**

**Figure 2: Optical conductivity measured in the infrared region under different temperatures and pressures.**

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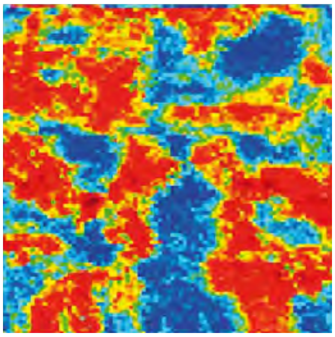

**Figure 3: Coexistence of metallic (red) and insulating (blue) phases observed by X-ray spectromicroscopy. The image covers an area of 50 x 50 µm².**

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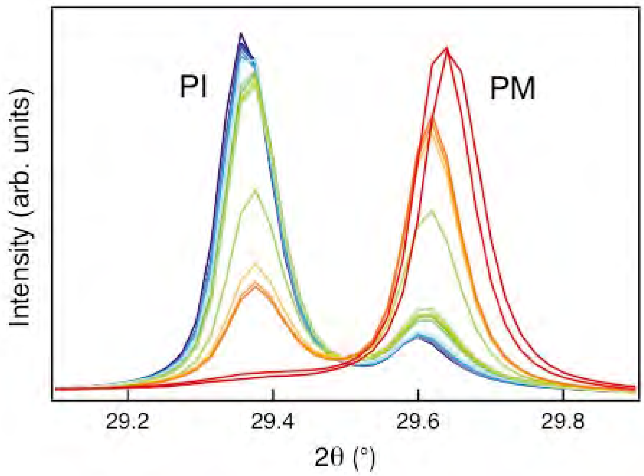



**Figure 4: The metal-insulator transition observed by X-ray diffraction. Starting from the insulating phase (PI, blue), only the metallic phase (PM, red) remains at high-pressure.**

the point considered in the "PM" region of the phase diagram: We can find a poor metal (blue curve, T = 220 K, x = 1.1%), a good metal (black curve, T = 300 K, x = 0) and intermediate cases (yellow and red curves). We confirmed these observations using the effective medium approximation (EMA) of the optical conductivity. These calculations showed that all spectra can be described by a mixture of various concentrations of metal and insulator. Thus, the «PM» spectrum measured at 220 K is composed of 45% metallic phase and 55% insulating phase, far from the image of a pure phase!

## Imaging the mixing of phases

It is even possible to directly visualize this mixing of electronic phases with X-ray spectromicroscopy, a technique which consists of measuring a photoemission spectrum at each point of the sample. The images obtained at ELETTRA and processed here in false colors, clearly show a coexistence of insulating and metallic phases on the microscopic level at the metal-insulator transition induced by temperature (blue and red zones in Figure 1). Even more surprising, the measurements show that the system keeps track of the pattern formed by the different phases, even after a complete cycle through the transition, probably due to the presence of Cr impurities that serve as nucleation centers.

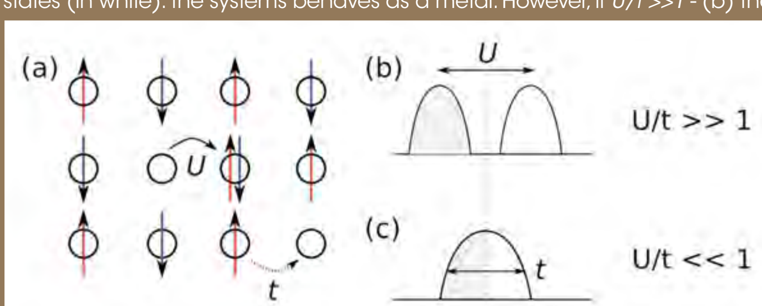
Phase mixing is particularly marked in the transition induced by temperature. In contrast, during the transition under pressure, the coexistence of phases observed indirectly by X-ray diffraction (Figure 4) on the CRISTAL beamline at SOLEIL, almost completely disappears at high pressure, leaving a more homogeneous and pure metallic phase. This result corroborates the optical conductivity measurements performed under pressure (Figure 2) which show growing metallic character as pressure increases.

## A combination of techniques is required

In conclusion, the measurements clearly evidence a mixing of metallic and insulating phases on the microscopic scale in $V_2O_3$, through the Mott transition induced by temperature, doping or pressure. The degree of purity of the metallic phase depends markedly on external parameters, but also on the impurities present in the sample. In general, this study highlights the complexity underlying the phase diagram of correlated materials and the need for a multimodal approach.

## The Mott transition

Like Kondo, Anderson, or de Gennes, Mott is one of the few eminent scientists who have lent their names to a physical effect that is still very relevant today. The Mott insulator model explains why some materials are insulators rather than conductors (metals) as expected from the filling of electronic shells, while the Mott transition focuses on the transition from one state to the other under the influence of external parameters (doping, pressure, temperature, etc.) The two phenomena are closely related to the Hubbard model that describes the behavior of an electron moving in an antiferromagnetic network (a). In this model, electrons can move from site to site through the hopping interaction t, identified to the electronic bandwidth. When a site is doubly occupied, it costs an extra energy U, the Coulomb interaction. It is the *U/t* ratio which determines the nature of the system: if *U/t* <<1 - (c), the electron band is half-filled (gray area) and the electrons are free to move by thermal excitations into the empty states (in white): the systems behaves as a metal. However, if *U/t* >>1 - (b) the interaction U opens up an energy gap that the electrons cannot cross. They are trapped: the behavior is that of an insulator, induced here by correlations.

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