

September 30th, 2010 - 10:00 am

Seminar Room 108, DESY Bldg. 49



Max Planck
Research
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for
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SEMINAR

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X-Ray Diffraction at High Pressures in $V_{1-x}Cr_xO_2$

VO_2 is a textbook example of strongly correlated material that has been extensively investigated in the last decades. A great source of interest is the fact that it undergoes a sharp metal-insulator transition coupled to a structural phase transition (from a rutile to a monoclinic M1 lattice) at 340°K whose underlying mechanism is still not fully understood [1,2]. Several models have been proposed, ranging from Peierls-type[3] to Mott-Hubbard-type[4] scenarios, stressing, to a different degree, the role of lattice instabilities and electronic correlations in driving the system towards the insulating phase.

In addition, when Cr impurities are added, weak rearrangements of the V-V chains lead to different monoclinic structures (M2 and M3) with only slight alterations of electronic properties [5].

Recently, high pressure measurements carried out by our group, coupled with infrared and Raman spectroscopy, pointed out that a novel high pressure monoclinic structure (named Mx) common for all the three different ambient pressure lattices (M1, M2, M3) exists above 10 GPa [6,7,8], where the system shows a bad metallic behaviour.

Since the monoclinic symmetry is, in principle, the signature of active Peierls distortions, the present results support a major role of the electron correlations against charge-lattice coupling in leading the MIT. However the role of the Peierls distortion in localizing free charges can not be completely ruled out.

In this talk, room temperature X-Ray powder diffraction data on $V_{1-x}Cr_xO_2$ collected at ESRF (Grenoble) over the 0–18 GPa pressure range for VO_2 , both pure and Cr-doped with two different concentrations ($x=0.007$, 0.025), will be presented. These measurements confirm our previous findings and allow the first structural characterization of these compounds for such high pressures. Starting from the three different ambient pressure structures (see Fig. 1-2) M1, M2, and M3 we observed that the patterns obtained evolve towards a striking similar high pressure one which exhibits some slight but important changes compared with the M1 ambient pressure pattern. Eventually, a phase diagram pressure vs doping will be illustrated.

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- [2] S. Biermann et al, Phys. Rev. Lett. 94, 26404 (2005)
- [3] J.B. Goodenough, J. Solid State Chem. 3, 490 (1971)
- [4] M. M. Qazilbash et al., Phys. Rev. B. 74, 205118 (2006)
- [5] J. M. Reyes et al., Can. J. Phys. 54, 413 (1976).
- [6] E. Arcangeletti, et al., Phys. Rev. Lett. 98, 196406 (2007)
- [7] C. Marini, et al., Phys. Rev. B 77, 235111 (2008)
- [8] C. Marini et al., High Pressure Res. 30, 55 (2010)

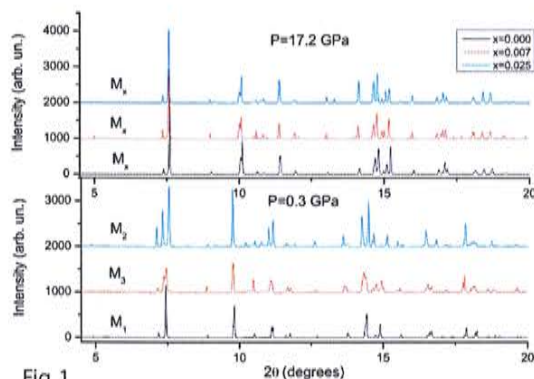


Fig. 1
X-ray diffraction pattern comparison at low ($P=0.3$ GPa) and high pressure ($P=17.2$ GPa).

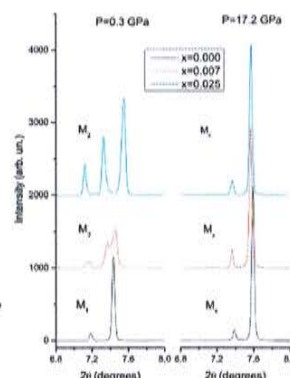


Fig. 2
Zoom of the main low angle reflections at low ($P=0.3$ GPa) and high pressure ($P=17.2$ GPa).



Host: Andrea Cavalleri, MPD