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# THERMODYNAMIC AND STRUCTURAL PROPERTIES OF WATER FILM ADSORBED ON MgO (100) SURFACE.



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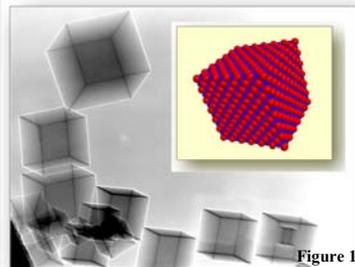


Figure 1

**Figure 1** : Transmission electron micrograph of our MgO powder sample, which is mainly composed of well defined nano cubes.

## Introduction

High homogeneous MgO (100) powder is a very suited substrate to investigate the influence of square symmetry surface on the properties of physisorbed rare gases (2D) films [1,2]. In addition, such a MgO (100) powder is of great interest to analyse the surface electric field influence on polar adsorbed monolayer (as for instance, NO, CO or C<sub>2</sub>H<sub>2</sub>). In the present study, we describe the thermodynamic and structural properties of (2D) water film physisorbed on MgO (100) surface. The structure of such (2D) water phase determined by neutron diffraction is commensurate P(2x3) and composed of water molecules chains (structure very similar to the (110) planes of the ice-VII, ice characterized by its high density  $d = 1.6$ ).

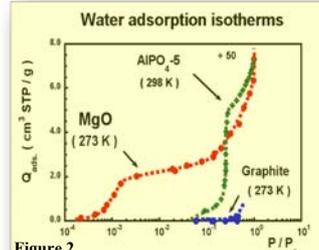


Figure 2

**Figure 2** : Adsorption isotherm measurements of water on MgO and graphite surfaces and AIPO4-5 zeolite.

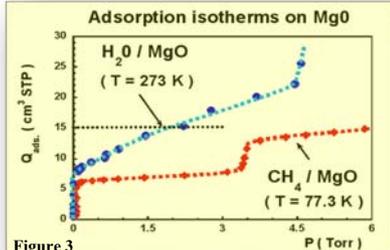


Figure 3

**Figure 3** : Calibration adsorption isotherm of water on MgO (100) powder measured at T = 273 K. By comparison, on the same MgO sample we have measured, a methane isotherm, at T = 77.3 K (the methane film is characterized by a square C(2x2) commensurate structure [3]).

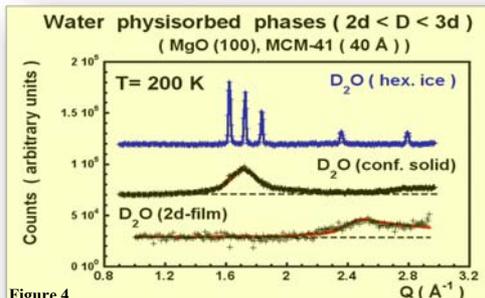


Figure 4

**Figure 4** : Neutron diffractograms of : (3D) hexagonal ice ; confined D<sub>2</sub>O solid phase in model MCM-41 (Ø = 40 Å) sample and D<sub>2</sub>O (2D) film adsorbed on MgO (100) surface at T = 200 K.

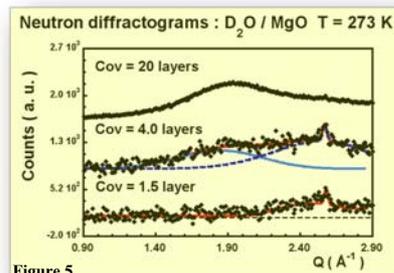


Figure 5

**Figure 5** : Neutron diffractograms of D<sub>2</sub>O adsorbed films on MgO (100) surface of different thicknesses : 1.5 layer ; 4.0 layers and 20 layers at T = 273 K.

**Results and discussion** : We have measured the neutron diffractograms of water (D<sub>2</sub>O) phase adsorbed on MgO (100) surface at different film thicknesses (0.93 ; 1.5 ; 4.0 and 20 layers). The determination of the water monolayer structure, from the analysis of the 0.93 layer diffractogram, was not so easy. In a first time, we start our analysis by considering water (2D) structure similar to the densest plane of hexagonal ice (Ih) and cubic ice (Ic). The results were not at all significant. In a second time, we have analyzed the structural properties of the high density ices (ices which exist in the high pressure domains). We have noted that, the main neutron diffraction peak of the cubic ice VII and the neutron diffraction signal of our 0.93 layer diffractogram are very close to each other (fig. 6a). Surprisingly, the densest plane of ice VII (plane (101)) is very close to the P(2x3) commensurate structure that we have already conjectured for the water monolayer structure [4]. In the present paper, we confirm such a P(2x3) over-structure mesh and we have determined the position and orientation of the water molecules within the mesh. The main characteristic of the (2D) water structural organization is that all the molecules are laying along the MgO (100) surface rows and form water molecular chains (as represented on fig. 7-8). To fit our measured neutron diffractograms (0.93 layer and 1.5 layer, as shown on fig. 4 and 5) we have considered the different morphology of such D<sub>2</sub>O chains (fig. 7).

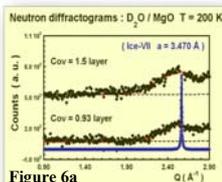


Figure 6a

**Figure 6a** : Neutron diffractograms of D<sub>2</sub>O films adsorbed on MgO (100) surface (0.93 and 1.5 layer) measured at T = 200 K in comparison with the diffractogram of ice-VII.

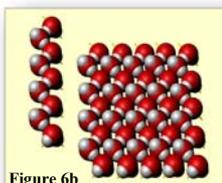


Figure 6b

**Figure 6b** : Schematic representation of the densest plane (101) of ice-VII. Such plane are composed of D<sub>2</sub>O chains. H-bondings between the planes insure the stability of the ice-VII structure.

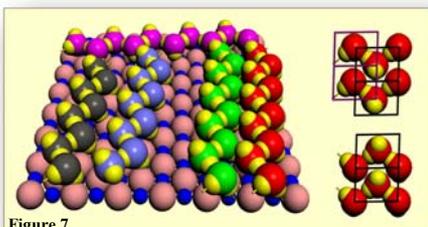


Figure 7

**Figure 7** : The water P(2x3) commensurate mesh contains 6 D<sub>2</sub>O molecules. In such a large mesh the water chains are characterized by different morphologies (12 morphologies). We have to consider such a disorder to fit our experimental diffractograms.

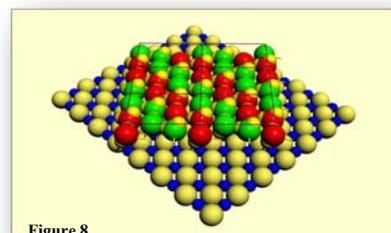


Figure 8

**Figure 8** : Schematic representation of the P(2x3) structure of water monolayer adsorbed on MgO (100) surface. We note that all the H<sub>2</sub>O molecules are laying along the surface rows formed by the Mg<sup>2+</sup> cations.

- References** : [1] J. P. Coulomb et O.E. Vilches, J. Physique (Paris) 45 (1984) 1381. [2] J.P. Coulomb, T.S. Sullivan and O.E. Vilches, Phys. Rev. B 30 (1984) 4753. [3] J.P. Coulomb, K. Madih, B. Croset and H.J. Lauter, Phys. Rev. Lett. 54 (1985) 1531. [4] B. Demirdjian, J. Suzanne, D. Ferry, J.P. Coulomb and L. Giordano, Surf. Science 462 (2000) L581.