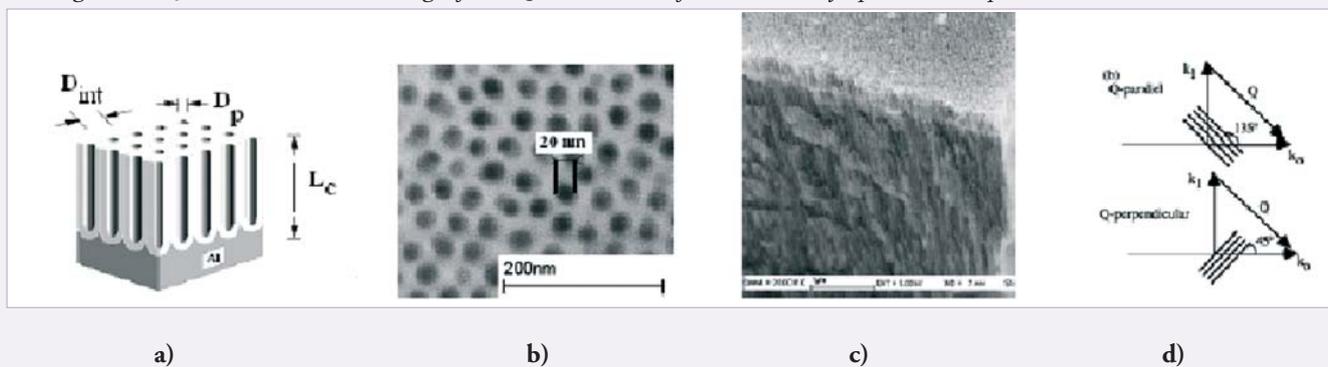


diameter,  $D_p$ , the inter-pores distance,  $D_{int}$ , and channels length,  $L_c$ . We have shown that the topology can be tailored so as to obtain fairly mono-disperse pores with diameter in the range 11 to 45 nm. The Small Angle Neutron Scattering (SANS) contrast matching technique is used to evidence that PEO can be fully and uniformly confined within the AAO porous network. We probe the properties of the confined polymer by differential scanning calorimetry and incoherent quasi-elastic neutron scattering. The ratio  $R_G / D_p$  sharply drives the properties of the confined polymer. Upon confinement, for  $D_p / R_G > 2$ , a strong depression of the melting point temperature is observed but above the bulk melting point the PEO dynamics is not affected. For  $D_p / R_G < 2$  no melting transition is detected and the PEO protons mean-square displacement is significantly reduced compared to the bulk behaviour.

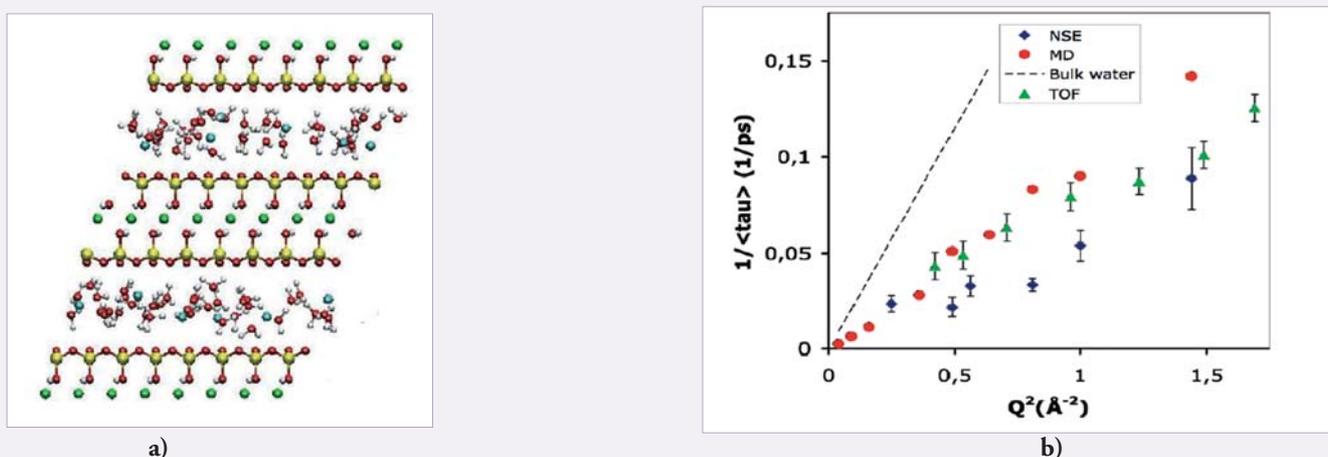
[K. Lagrené and J.-M. Zanotti, *Proceedings of the QENS 2006 conference, MRS Symp. Proc., accepted.*]



**Figure 1.** a) Schematic drawing of a porous alumina membrane. b) Scanning Electron Microscope (SEM) image of a LLB made AAO membrane. Here, the pore diameter is 20 nm. c) 3D SEM view of an actual LLB made AAO membrane showing the macroscopic alignment of the cylindrical pores in the bulk of the membrane (scale is 1  $\mu\text{m}$ ). d) Schematic illustration of how relative orientation of AAO samples to the incident beam ( $k_0$ ) and measurement of the intensity scattered in a detector at  $2\theta = 90^\circ$  (i.e. along  $k_1$ ), can provide information (sensed along  $Q$ ) on confined PEO dynamics parallel (top) and perpendicular (bottom) to the AAO cylinders axes.

### [C3. N. Malikova] Dynamics of water and ions in clays: a concurrent TOF, NSE and MD study

The potential application of clays as components of barriers around underground storage sites of radio-active waste has recently intensified the study of mobility of water and ions (both natural, e.g.  $\text{Na}^+$ , and potential radionuclides, e.g.  $\text{Cs}^+$ ) in these systems. At a more fundamental level, these investigations shed light onto dynamics of liquids in confined charged media and phenomena at a solid/liquid interface. The dynamics of water in a montmorillonite clay has been investigated here on the picosecond timescale by quasi-elastic neutron scattering (time-of-flight (TOF) and neutron spin echo (NSE) techniques) and classical molecular dynamics (MD) simulations.



**Figure 1.** a) Atomic structure of a hydrated clay used in MD. Mobile species: water molecules (white and red),  $\text{Na}^+ / \text{Cs}^+$  ions (blue). b) Inverse relaxation times versus the wave-vector for two-layer hydrate of Na-montmorillonite.

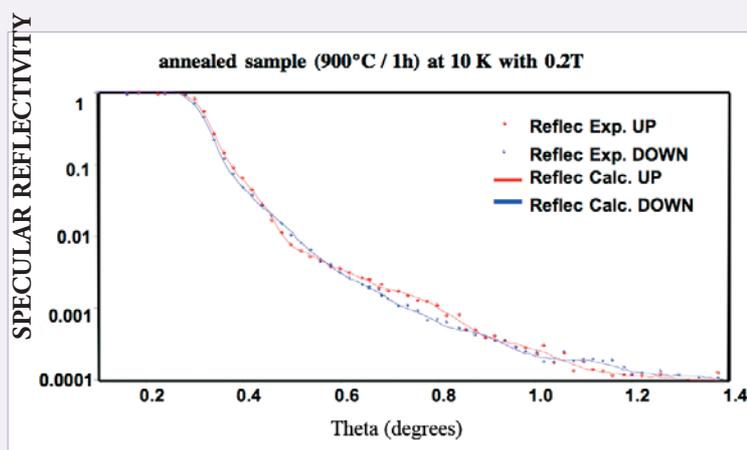
MD shows that while  $\text{Na}^+$  ions have no specific adsorption sites on the clay surface,  $\text{Cs}^+$  ions exhibit a jump diffusion between sites allowing coordination to six oxygen atoms of the adjacent clay layers. In the bulk, on the picosecond-nanosecond timescale, water molecules diffuse by a combination of translational and rotational motion. In the case of clays, this behaviour is necessarily modified by the narrow confinement between two parallel clay layers. Never-the-less, while the water diffusion coefficient in case of a single confined water layer is an order of magnitude lower than in bulk water ( $1-2 \times 10^{-10} \text{ m}^2/\text{s}$ ), in the two-layer clay hydrate the diffusion coefficient is already almost half of the bulk value ( $1 \times 10^{-9} \text{ m}^2/\text{s}$ ,  $D_{\text{bulk}}=2.3 \times 10^{-9} \text{ m}^2/\text{s}$ ). This is seen both in experiment and simulation.

*PhD thesis of N. Malikova (LI2C/ANDRA), [Collaboration LI2C (Université P&M Curie, Paris VI, CNRS) and LLB ] Malikova, Cadène, Marry, Dubois & Turq, J. Phys. Chem. B 110, pp.3206-3214, 2006.*

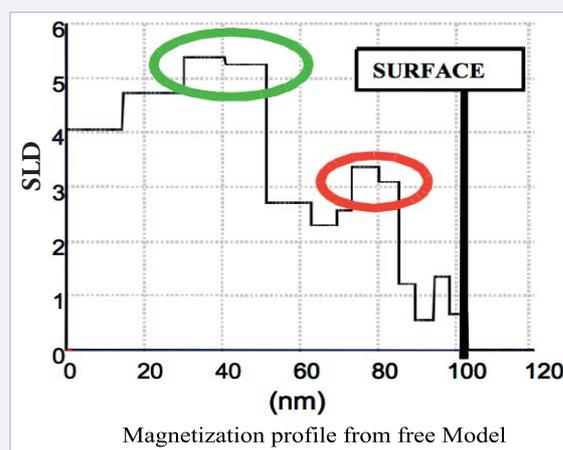
#### [C4. A. Declémy] Ferromagnetic Fe-implanted SiC: New results towards a Diluted Magnetic Semiconductor

SiC is a good candidate for diluted magnetic semiconductors which could be used in spin-electronic devices. It has a wide band-gap (3.1 eV), low spin-orbit coupling, excellent transport properties and has reached a mature state of industrial development. In order to create magnetic SiC, substrates have been implanted with Fe ions at the LMP Univ. Poitiers (at doses of the order of  $5.10^{16}/\text{cm}^3$ ). After annealing (700-900°C), a ferromagnetic behavior has been observed with a high Curie temperature (up to 700°C). Polarized neutron reflectivity has allowed to probe the magnetization of the SiC:Fe films as a function of the depth. From the PNR reflectivity (Fig. 1), it is possible to reconstruct the magnetization profile (Fig. 2). The complicated shape of the fitted magnetization profile through the depth of the sample is connected to the multi-implantation process. The measured profile corresponds quite well with the implantation profile which can be simulated with SRIM. The fact that we are dealing with a magnetic semi-conductor needs to be confirmed. Until now, EXAFS shows that there are no Fe atoms in the very near Fe environment which excludes the presence of Fe clusters. The possibility of secondary phases such as  $\text{Fe}_3\text{Si}$  needs to be checked.

*[Collaboration: A. Declémy, M. Drouet, C. Dupeyrat, D. Babonneau, J. Mimault, T. Girardeau, D. Eyidi, M.F. Beaufort, J.P. Eymery, Université de Poitiers, F. Ott, M. Viret, LLB/SPEC Saclay.]*



**Figure 1:** polarized neutron reflectivity of an SiC:Fe sample measured at 10K (fits in solid lines)



**Figure 2:** Reconstruction of the Fe implantation profile from the PNR. The fit is very close to the calculated implantation profile

#### [C5. V. Klošek] A compact tensile machine for in situ neutron diffraction study of materials under external loading

In order to characterize the behaviour of materials under mechanical loading, a very compact tensile machine was recently developed at LPM TM. This machine is designed to be mounted on the Eulerian cradles of G5.2 and 6T1 diffractometers: to allow a huge variety of sample orientations, its frame consists in two side columns on which are fixed the plates supporting the tensile heads (Fig. 1). It thus now becomes possible to analyse elastic and plastic behaviours of materials during a tensile test by in situ neutron diffraction. This machine is an incomparable tool to study deformation mechanisms under external loading of materials: macro- and micro-strains, texture or stored energy can now be measured as a function of applied load (up to 30 kN). First tests were performed on a brass (Cu-Zn) alloy sample. Figure 2 shows the (111) diffracted peaks recorded on G5.2 at three different loadings, with their corresponding FWHM ( $\lambda = 3.03 \text{ \AA}$ ). At low strain, the peak is essentially shifted toward lower angles (elastic deformation mainly). At higher strain, the peak broadens, traducing the plastic deformation of the material.