MD shows that while Na+ ions have no specific adsorption sites on the clay surface, 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 ¥ 10-10 m2/s), in the two-layer clay hydrate the diffusion coefficient is already almost half of the bulk value (1 ¥ 10-9 m2/s, Dbulk=2.3 ¥ 10-9 m2/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 $5.10^{16}/cm^3$). 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 Fe3Si 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.]

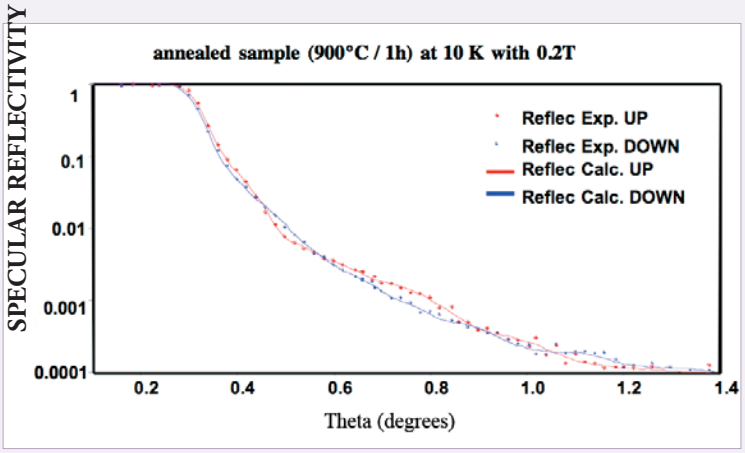

Figure 1: polarized neutron reflectivity of an SiC:Fe sample measured at 10K (fits in solid lines)

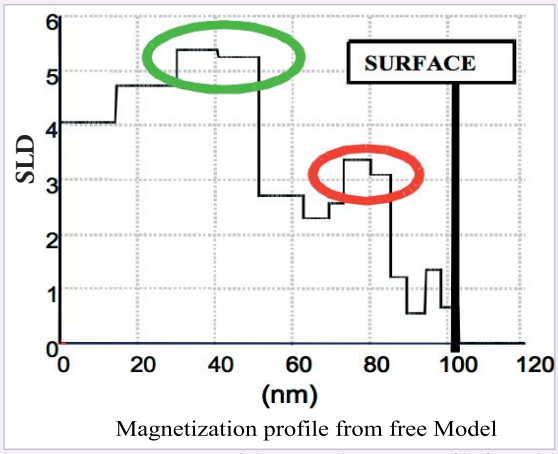

Figure 2: Reconstruction of the Fe implantation profile from the PNR. The fit is very close to the calculated implantation profile

[*C5.* V. Klosek] **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 LPMTM. 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 (λ = 3.03 Å). 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.