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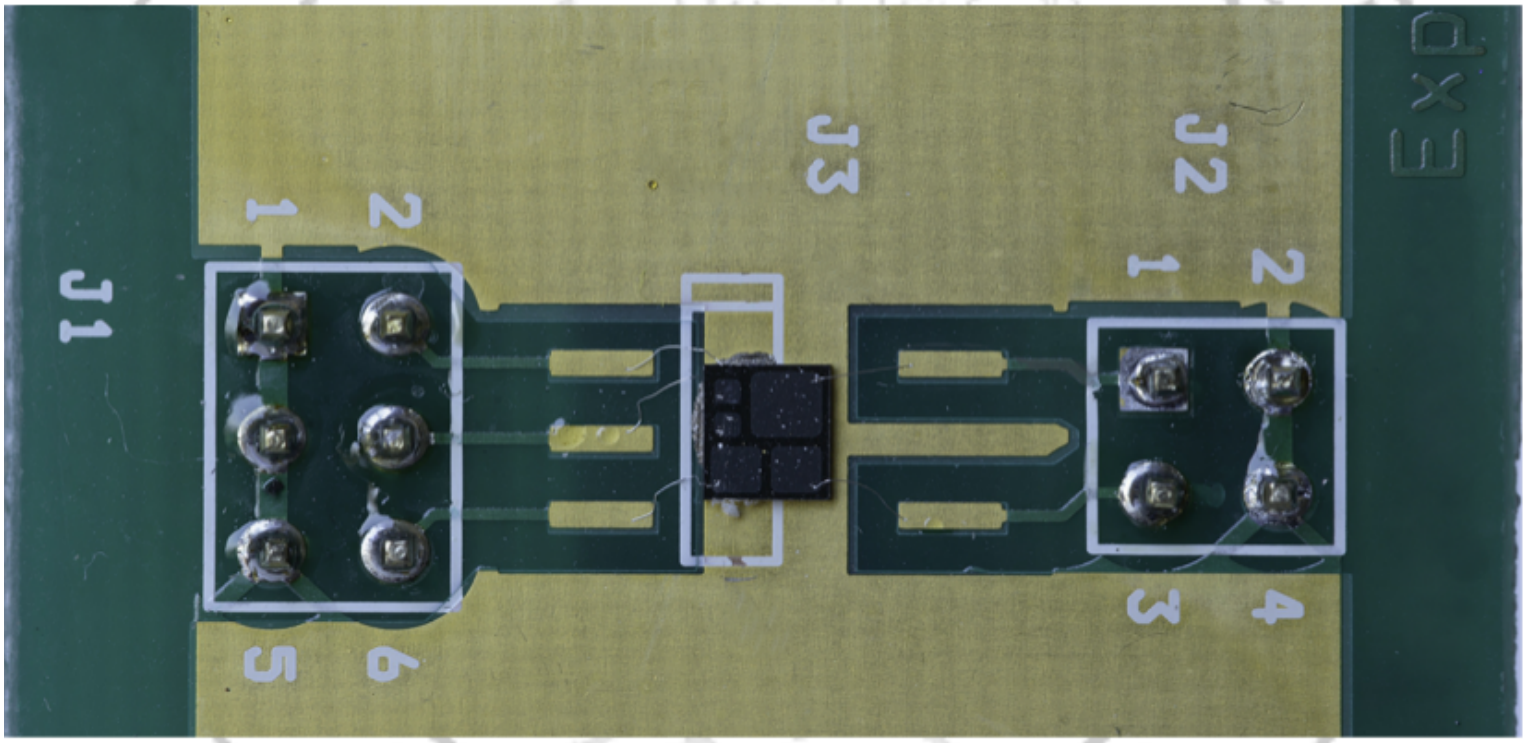
DOTTORATO DI RICERCA IN FISICA
UNIVERSITÀ DI MESSINA



ACTIVITY REPORT
2014

C/O DIPARTIMENTO DI FISICA

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DOTTORATO DI RICERCA IN FISICA
UNIVERSITÁ DI MESSINA

ACTIVITY REPORT
2014

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C/O DIPARTIMENTO DI FISICA
E DI SCIENZE DELLA TERRA

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RIORDINO DELLA NORMATIVA DEL DOTTORATO DI RICERCA

L. Torrisi

Coordinatore del Dottorato di Ricerca in Fisica dell'Università degli Studi di Messina

Il dottorato di ricerca è stato istituito in Italia nel 1980 (d.P.R. 11 luglio 1980, n. 382, Capo II, artt. 68 ss.) come "titolo accademico valutabile unicamente nell'ambito della ricerca scientifica". Tra la fine degli anni '90 e l'inizio degli anni 2000, in consonanza, da un lato, con i principi dell'autonomia delle università, dall'altro, con gli indirizzi europei (Processo di Bologna, 1999; Principi di Salisburgo, 2005), si fece sentire urgente la necessità di una sua revisione.

Da un sistema normativo prevalente espressione del centro statale, si passò così (l. 3 luglio 1998, n. 210, art. 4; d.m. 30 aprile 1999, n. 224; d.m. 3 novembre 1999, n. 509; d.m. 22 ottobre 2004, n. 270) a una scarna disciplina di principio che lasciava interamente alle università la responsabilità dell'organizzazione dei corsi di dottorato. Inoltre si individuò chiaramente il dottorato di ricerca come terzo ciclo della formazione superiore e, al contempo, come primo stadio dell'attività di ricerca - il dottorando come early stage researcher - riconoscendogli un ruolo strategico nell'alta formazione delle giovani generazioni e nello sviluppo del Paese.

Un nuovo cambiamento, ispirato a una visione più centralistica e collegato al tema della valutazione, è stato apportato dall'articolo 19 della legge 30 dicembre 2010, n. 240, e dai conseguenti provvedimenti applicativi – il regolamento per l'accreditamento (d.m. 8 febbraio 2012, n. 45), le relative Linee guida (nota ministeriale n. 436 del 24/3/2014), il documento ANVUR del 24 luglio 2014 sulla valutazione dei corsi di dottorato – alcuni ancora in fase di elaborazione definitiva.

Il dottorato, oltre a essere il luogo di maturazione per le nuove leve di studiosi delle università e degli enti di ricerca, deve anche avere l'ambizione di formare alla ricerca e, per suo tramite, alle alte professionalità del mondo del lavoro, giovani che sappiano essere motore di trasferimento di conoscenza e innovazione nelle imprese, nella pubblica amministrazione, nelle professioni e in tutte le attività produttive. Può anche costituire una risorsa significativa per il lifelong learning dei quadri dirigenti del mondo del lavoro.

Per queste caratteristiche il dottorato costituisce un segmento formativo particolare che richiede flessibilità e ricchezza di percorsi, così da potersi adattare alle esigenze molteplici di realtà diverse e in continua evoluzione. Il dottorato è inoltre uno dei fattori importanti della qualità complessiva di un'università e della sua ricerca. Le università, quindi, devono poter organizzare i loro corsi di dottorato secondo le loro tradizioni e le loro vocazioni di ricerca, e perseguirne la qualità in piena autonomia.

D'altra parte la qualità dei risultati ottenuti deve essere valutata regolarmente e in modo stringente anche dai portatori di interesse, in primo luogo lo Stato, così da poter monitorare e indirizzare gli investimenti e da spingere gli atenei a raggiungere e mantenere nel tempo un alto livello qualitativo dell'offerta dottorale.

La normativa introdotta dagli articoli 5, comma 3, e 19, comma 1, della legge 240/2010 affida il compito di regolare il dottorato di ricerca ad un sistema nazionale di accreditamento e valutazione.

L'accreditamento è fondato "sull'utilizzazione di specifici indicatori, definiti ex ante dall'ANVUR, per la verifica del possesso da parte degli atenei di idonei requisiti didattici, strutturali, organizzativi, di qualificazione dei docenti e delle attività di ricerca, nonché di sostenibilità economico-finanziaria". La valutazione periodica è fondata "su criteri e indicatori stabiliti ex ante, da parte dell'ANVUR, dell'efficienza

e dei risultati conseguiti nell'ambito della didattica e della ricerca dalle singole università e dalle loro articolazioni interne".

Inoltre l'articolo 3 del DM 45/2012 specifica che l'accreditamento si articola "nell'autorizzazione iniziale" e "nella verifica periodica della permanenza dei requisiti richiesti per l'accreditamento" iniziale. Il decreto dedica invece meno spazio alla valutazione, che vi compare solo nell'articolo 13 su "valutazione e finanziamento dei corsi di dottorato".

In tutte le migliori realtà internazionali l'accreditamento periodico dei corsi è il risultato della verifica congiunta del possesso di alcuni requisiti fondamentali e, soprattutto, degli esiti di una valutazione della qualità dei risultati ottenuti, mediante le procedure dell'autovalutazione e della valutazione esterna con visite in loco, come del resto è prescritto dall'articolo 3 del DPR 76/2010 e come avviene nel sistema AVA di accreditamento dei corsi di laurea e di laurea magistrale.

Il Dottorato XXX Ciclo dell'Università di Messina è stato giudicato favorevolmente da parte dell'Agenzia Nazionale di Valutazione del Sistema Universitario e della Ricerca (ANVUR). Il Giudizio, ampiamente positivo, ha riguardato in particolare la valutazione dei seguenti parametri:

Requisito A.1 Qualificazione scientifica della sede del dottorato
Requisito A.2 Tematiche del dottorato ed eventuali curricula
Requisito A.3 Composizione del collegio docenti
Requisito A.4 Qualificazione del collegio dei docenti
Requisito A.5 Numero borse di dottorato
Requisito A.6 Sostenibilità del corso
Requisito A.7 Strutture operative e scientifiche
Requisito A.8 Attività di formazione

Quest'anno, a causa dell'entrata in vigore della nuova normativa, col XXX Ciclo il Dottorato di Ricerca in Fisica accoglie, presso il Dipartimento di Fisica e Scienze della Terra dell'Università di Messina, dottorandi partecipanti ai seguenti cicli:
XXX Ciclo: 6 dottorandi in corso, tutti con borsa, con inizio di attività dal 1° Novembre 2014;
XXIX Ciclo: 6 Dottorandi in corso con fine attività il 30 Settembre 2016;
XXVIII Ciclo: 3 Dottorandi, di cui una straniera, in corso con fine attività il 31 Dicembre 2015;
XXVII Ciclo: 5 Dottorandi in corso con fine attività il 31 Dicembre 2014.
Erasmus Mundus-Emmag: 1 Dottorando Algerino.

Il Collegio dei Docenti è stato costituito da 45 membri, di cui 16 facenti parte del Collegio ristretto. L'attività formativa si è basate su lezioni, di carattere generale e specialistico, e cicli di seminari.

Ogni anno viene pubblicato l'Activity Report in cui si raccolgono i lavori di tutti gli studenti del Dottorato di Ricerca in Fisica.

Il Coordinatore
Prof. Lorenzo Torrisi

REPORTS

PhD STUDENTS
CYCLE XXVII

McStas simulation on IN5 spectrometer following RENS approach

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Abstract

In this paper the results of a simulation study by the software package McStas on IN5 spectromerer operating following the Resolution Elastic Neutron Scattering (RENS) approach are reported. The McStas neutron ray-tracing software package is a tool for accurate simulations of neutron scattering instruments at reactors, short- and long-pulsed spallation sources such as the European Spallation Source (ESS). The RENS approach consists in measuring the Elastically Incoherent Neutron Scattering (EINS) intensity versus the instrumental energy resolution $\Delta\omega_{RES}$. It is shown that the EINS intensity versus the logarithm of $\Delta\omega_{RES}$ gives rise to an increasing sigmoid trend whose inflection point occurs when the instrumental energy resolution value corresponds to the system relaxation time.

Keywords: Resolution Elastic Neutron Scattering, McStas, Simulation.

Introduction

It is well known that thermal neutrons, which have $10^{-}1 \div 10, \mathring{A}$ wavelengths and energies in the meV ranges, constitute a probe able to characterize the material systems dynamical properties; this is made possible thanks to: i) the time-space scale to which they are sensitive; ii) the simplification brought about by the neutron-nucleus interaction; and to iii) the neutron distinctive isotopic character which allows to highlight the contribution of different portion of the sample. On that score, the characterization of the molecular motions can be effectively performed by EINS , through the so called fixed-windows method. The aim of this work is to present first results of a McStas simulation on RENS, this latter being an approach based on the acquisition of the measured elastic scattering law as a function of the instrumental energy resolution In particular it is shown that the measured elastic scattering law as a function of the logarithm of the instrumental energy resolution $\Delta\omega_{RES}$ behaves like an increasing sigmoid curve whose inflection point occurs when the instrumental resolution time matches the system relaxation time. The behaviour of a neutron scattering instrument can be described by a complex integral over all relevant parameters, like initial neutron energy and divergence, scattering vector and position in the sample, etc., thanks to the Monte Carlo Simulation of Triple Axis Spectrometer (McStas) package which allows to simulate an experiment. In particular, McStas package is a flexible tool for building accurate simulations of neutron scattering instruments at reactors, short- and long-pulsed spallation. In particular, McStas can be extensively employed for:

- designing new instruments,
- optimizing existing instruments,
- improving usage of existing instrument,
- getting accustomed with the instruments before experiments,
- comparing virtual experiments with real ones, also during the experiments
- estimating complex effects like: absorption, geometry, multiple scattering and resolution function.

McStas was founded as a scientific, open-source collaborative code in 1997; it has an open-source, collaborative nature designed to use component codes written by scientists, later to be shared via the McStas component library. In McStas these small and medium sized component-codes implement the individual parts of a beamline. McStas users need not write components themselves, but always have the option to do so when a component is missing or needs improvement. For the user operating McStas only knowledge of a simple instrument file containing a logical and easy to read meta-language is needed [1]. The McStas software suite then translates the instrument file into a computation-effective and portable c-code using powerful code-generation and compiler techniques. One other strong point is the availability of sample components, allowing the user to perform a Virtual Experiment [2], where one combines sample and instrument response to give a close-to-physical virtual dataset as output. Today, McStas has an impressive suite of components in all categories, counting 148 pieces of code, out of which

around 40are user contributions. Further, 100 example instruments gives the new user rich inspiration for own projects. In this work the IN5 spectrometer has been taken into account for the simulation with McStas. IN5 is a high precision direct geometry Time of Flight (ToF) spectrometer, which is addressed to study low-energy transfer processes as a function of momentum transfer. Typically this instrument is used for measurements in the small energy range of $10\mu eV$ to 100 meV, in the wavevector range of $1.8\mathring{A}$ to $20\mathring{A}$ and a chopper velocity (revolution per minute) of $2000rpm$ to $17000rpm$. IN5 is constituted by a series of guides, chopper and collimators, which accompany the neutron beam from the source to the sample. The neutrons diffuse along a series of optical guides, which avoid the dispersion of the beam; their path is 17 meters.

Material and method

From the formal point of view the scattering law $S(Q,\omega)$ and the intermediate scattering function $I(Q,t)$ are directly connected through time Fourier transform [3]-[8]:

$$S(Q,\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} I(Q,t)e^{-i\omega t}dt \qquad (1)$$

$$I(Q,t) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} S(Q,\omega)e^{i\omega t}d\omega \qquad (2)$$

As above noticed, these functions make reference to the system properties and not to the measured quantities; in fact, it should be taken into account that, for example, when the experimental technique gives access to the scattering law one should take into account the less straightforward connection with the measured scattering function, which is the convolution of the scattering law with the instrumental resolution function, i.e.:

$$S_R = S(Q,\omega) \otimes R(Q,\omega) \qquad (3)$$

By the convolution theorem Eq. 3 can be written as:

$$S_R(Q,\omega) = \frac{1}{\sqrt{2\pi}}\int_{+\infty}^{-\infty} I(Q,t)\cdot R(Q,t)dt \qquad (4)$$

More generally, the experimentally measured elastic scattering law, due to the finite energy instrumental resolution $\Delta\omega$, $S_R^M(Q)$ is:

$$S_R^M(Q) = \int_{+\frac{\Delta\omega}{2}}^{-\frac{\Delta\omega}{2}} S_R(Q,\omega)d\omega \qquad (5)$$

and hence:

$$S_R^M = \int_{-\frac{\Delta\omega}{2}}^{+\frac{\Delta\omega}{2}} \left[\frac{1}{\sqrt{2\pi}}\int_{+\infty}^{-\infty} I(Q,t)\cdot R(Q,t)cos\omega t dt\right] d\omega. \qquad (6)$$

In order to simulate the behaviour of the IN5 instrument following the RENS approach McStas was employed. In this framework in McStas the monochromatic neutron source can be continuous or pulsed. The optic can be moving or static. The moving optics take into account the choppers (disk and Fermi), the velocity selectors and the phase space transformers. Whereas the static optics considers the guides, the mirrors, the benders, the lenses, collimators, slits, filters and monochromator. The samples that can be simulated are single crystals, liquid, gas, polymers and hard spheres. As far as the detectors are concerned, they take into account histograms and event monitors or gas detectors. Structurally, McStas consists of several layers and types of code. Many elements of the code can be manipulated, the other elements belonging to systems parts of McStas [9]-[10]. More precisely:

- the user defines the instrument using the mcgui program on the "tool layer", thereby assembling a so-called instrument file containing a logical and easy to read meta-language, positioning components of the beamline in a coordinate frame. The lab- or instrument coordinate system is right-handed, with y defining the vertical axis and z the direction of the neutron beam.
- Each of the components correspond to a McStas component file in the component library, written in a type of structured C-code. A user does not need to write component files, but has the option to do so. The components each have their local coordinate frame in which the neutron should be propagated between an incoming and outging state, e.g. before and after a scattering process. The McStas system takes care of transformation of the neutron state from one component coordinate system to the next.
- From the instrument code, the component codes and special kernel/runtime code containing e.g. a random number generator, propagation routines and physical constants, a computation-effective and portable c-code is generated by the McStas system using a powerful code-generation and technique. Further, a c-compiler is called, generating a binary executable, typically referred to as the simulation. These two steps happen transparently and without user interaction.
- Following the compilation process, the simulation can be run to produce output data, in the

form of event data files, histograms or an interactive visualization of the instrument geometry. The tools layer contains the tools mcplot and mcdisplay, for histograms and instrument geometry data respectively.

In Fig. 1 a sketch of a simulation workflow in McStas.

Figure 1: *Illustration of a simulation workflow in McStas.*

Result and discussions

Following the RENS approach one has to take into account an increasing instrumental resolution function linewidth $\Delta\omega_{RES}$ and then to apply eqn. 6 for determining the value of the definite integral as a function of $\Delta\omega_{RES}$. Figure 2 shows the result of such a calculation, i.e. S_R^M as a function of temperature and as a function of logarithm of the instrumental resolution. What it clearly emerges is that it shows in both the case a sigmoid trend with an inflection point which occurs when the linewidth of the resolution function approaches the linewidth of the system scattering law; in other words the inflection point occurs when the instrumental resolution time crosses the system relaxation time. Such results show the operating way of the EINS versus temperature and RENS versus instrumental energy resolution approach: from the inflection point of EINS profiles versus temperature and versus the logarithm of the energy resolution one can extract the system relaxation time. In fact, in a complementary way, for a given fixed instrumental energy resolution function, from EINS profiles versus temperature one is able to obtain, from the inflection point, the temperature value for which the system relaxation time equals the resolution time.

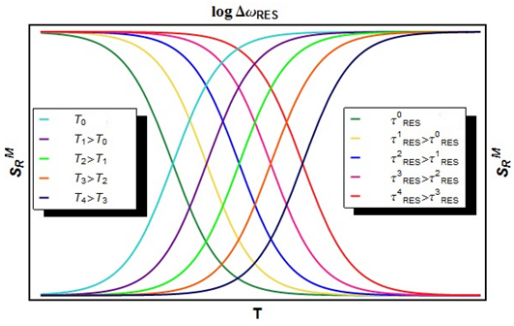

Figure 2: *A comparison between measured elastic scattering law vs. $\Delta\omega_{RES}$ for different temperature values and measured elastic scattering law SRM vs. T for different instrumental energy resolution values.*

In this work a simulation of the IN5 spectrometer operating following the RENS approach is performed by means of McStas by varying the value of wavelengths and considering different values speeds of the chopper. As an example in the following table two employed instrument parameters are reported:

INSTRUMENT'S SETTING					
lambda	4.18 Å	**dlambda**	4 Å	**speed**	2000rpm 5000rpm
ratio	0.5	**housing**	Fe.laz	**coh**	V.laz
inc	null	**thickness**	1 mm	**height**	2.5 mm
radius	5 mm		**order**	multiple scattering	
Neutron count			500000000		

Figure 3: Employed instrument parameters values

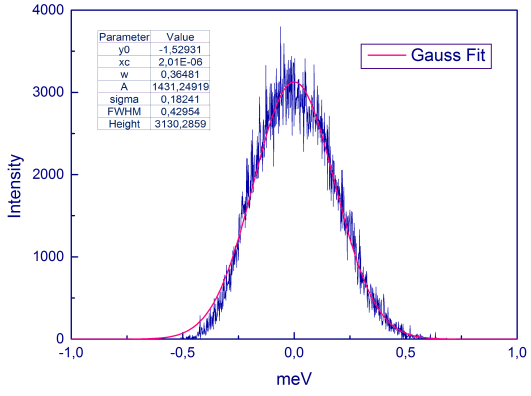

Figure 4: *Simulated dynamical structure factor for Vanadium.The incoming wavelength is: 4.18Å; the chopper speed is: 2000 rpm; FWHM is: $\Delta E 358.15 \mu eV$.*

Fig.4 shows a simulated dynamical structure factor for Vanadium as obtained by keeping constant the thickness of the sample: 1 mm and the incoming wavelength spread $\Delta\lambda$: 4$\mathring{A}$. The incoming wavelength is: 4.18$\mathring{A}$; the chopper speed is: 2000 rpm; the neutron counts are fixed to 500.000.000; the speed ratio between chopper 3 and chopper 1 is 0.5. The obtained Gaussian like curve, whose width has been extracted through a fitting procedure by means of the ORIGIN 9.0 version, shows Full Width at Half Maximum (FWHM) of ΔE358.15μeV.

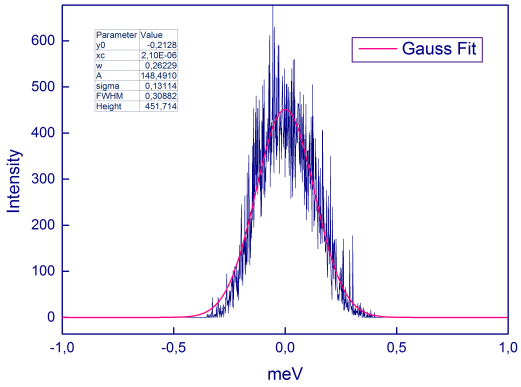

Figure 5: *Simulated dynamical structure factor for Vanadium.The incoming wavelength is:* 4.18$\mathring{A}$*; the chopper speed is: 5000 rpm; FWHM is:*ΔE308.82μeV.

Fig.5 shows a simulated dynamical structure factor for Vanadium as obtained by keeping constant the thickness of the sample: 1 mm and the incoming wavelength spread $\Delta\lambda$: 4$\mathring{A}$. The incoming wavelength is: 4.18$\mathring{A}$; the chopper speed is: 5000 rpm; the neutron counts are fixed to 500.000.000; the speed ratio between chopper 3 and chopper 1 is 0.5. The obtained Gaussian like curve, whose width has been extracted through a fitting procedure shows FWHM of ΔE308.82μeV.

Conclusions

A varying instrumental energy resolution, and a varying energy window as well, allow to characterize the motion characteristic times. Following the RENS approach the measured elastic scattering law as a function of the logarithm of the instrumental energy resolution shows an inflection point when the instrumental energy resolution coincides with the system relaxation time. In this contribution first results of a McStas 2.1 simulation operating following the RENS approach are reported. The obtained Gaussian like curves show FWHM values in agrrement with IN5 instrument features.

References

[1] Lefmann, K., Nielsen, K. Neutron News **10**, 1999, p.20

[2] Lefmann, K. et al., J. Neut. Res. **16**, 2008, pp. 97-111

[3] Van Hove, L. Phys. Rev. **84**, 1954, p.249

[4] Volino, F. *Spectroscopic Methods for the Study of Local Dynamics in Polyatomic Fluids.* Plenum, New York, 1978.

[5] Rahman, A., Singwi, S., Sjolander, A. Phys. Rev. **84**, 1962, p.986

[6] Magazú, S., Migliardo, F., Telling, M.T.F. Food Chem. **106**, 2008, p.1460

[7] Magazú, S., Migliardo, F. Affouard, F., Descamps, M., Telling, T.F. J. Chem. Phys. **132**, 1960, p.123

[8] Migliardo, F., Caccamo, M.T., Magazú, S. J Non-Cryst. Sol. **378**, 2013, p. 144

[9] Willendrup, P., Filges, U., Keller, L., Farhi, E., Lefmann, K., Phys. B-Cond. Matt. **385**, 2006, p. 1032

[10] Knudsen, E.B., Udby, L., Willendrup, P., Lefmann, K., Bouwman, W.G. Phys. B-Cond. Matt. **406**, 2011, p. 2361

Diffusion in DMPC-octanol bilayers

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Abstract

Phospholipid bilayers are very complex systems, characterized by auto-organized dynamics that are very important for biochemichal reactions of life cell. In this study we discuss how alcohol inserction influences phospholipid bilayer dynamics, through analisys of MD simulation.

Keywords: biomimetic membrane, MD, lipid raft.

Introduction

Membrane is the basic organ in the constitution of cells. It defends and separates cell from external environment, assuring ideal conditions to biochemistry of life. Through the particoular membrane structure the cell is able to have a selective interaction with environment; mobility of its constituents permits an optimal adapting capability to different external conditions. Particularly important for bilayer dynamics it is presence of so-called *lipid rafts*, *i.e.* phospholipid aggregates that moves as a single functional unit, transporting specific molecules through cellular membrane.

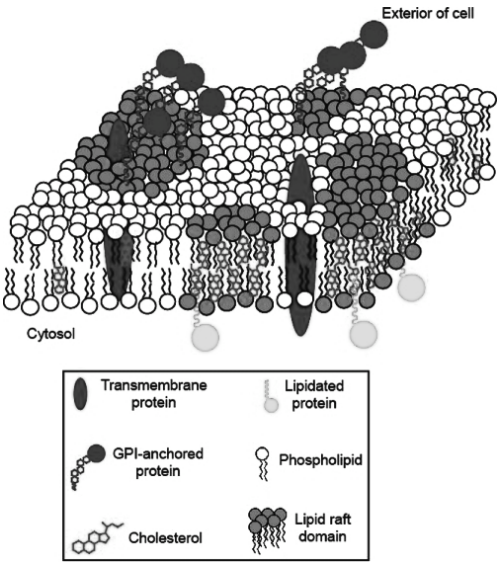

Figure 1: *Bilayer with lipid rafts*

The central core of any biological membrane is formed by phospholipids, amphiphilic molecules composed of two fatty acids, a glycerol unit, a phosphate group and a polar molecule. The phosphate group and polar head region of the molecule is hydrophilic, while the fatty acid tail is hydrophobic. When placed in water, phospholipids will orient themselves side by side to form a lipid bilayer with head groups turned towards the surrounding water and apolar acyl chains in the membrane interior.

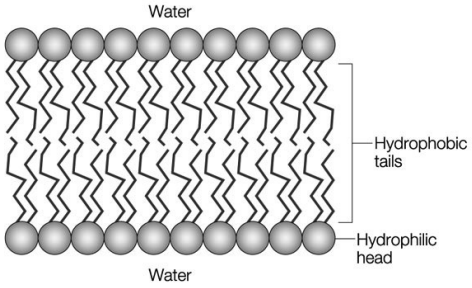

Figure 2: *Phospholipid bilayer structure*

Because their complex structure, this molecoular bilayers are caracterised by a variety of dynamics centered about different temporal ranges. Natural membranes are too complex systems to be investigated by physical techniques in order to understand the relationship between the structure and dynamics of the system and the membrane functions. A simpler model membrane can then be realized by an artificial assembly of one type of phospholipid arranged in a multi-bilayer structure in an aqueous environment. This simple model can be complessified by adding different types of molecules in bilayer composition.

Alcohol influences on bilayer in particular are an interesting matter of study: it is known by literature as alcohols have anaesthetic properties. There were several mechanisms proposed to explain the molecular interactions that cause anaesthesia. But they are not able to give a clear picture about the molecular mechanism. Nevertheless most of the proposed theories revolve around anaesthetics influence on the membranes. It is believed that anaesthetics may be directly act upon the receptors or indirectly influence them by perturbing the lipid membranes. Some believe the membrane to be the site of anaesthetic action, and others believe that proteins are the sites of anaesthetic action. Studying alcohol influences on phospholipid dynamics could give us new elements to estabilish effetive role of this molecules ad anaesthetic[3, 4].

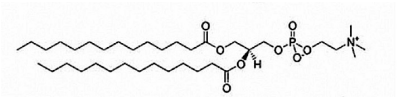

Figure 3: *1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC)*

Figure 4: *Octanol*

MD analisys and Results

MD trajectory was implemented through NAMD package. System analyzed is a DMPC-octanol bilayer ratio 1:2 in aqueous environment (see tab 1 for details); trajectory covers 4 ns temporal range.

Table 1: *Simulated sample composition*

DMPC	64
Octanol	32
Water	4474

By analisys of system MD we report two observations:
1) It is possible to notice that collective motions that can be easily observed in simulation of single-lipid bilayers [2], aren't further visible in systems composed by octanol and DMPC; this fact suggests that contemporary presence of molecules with a non-negligible difference in volumes causes a destruction of coherent dynamics (see fig. 5).

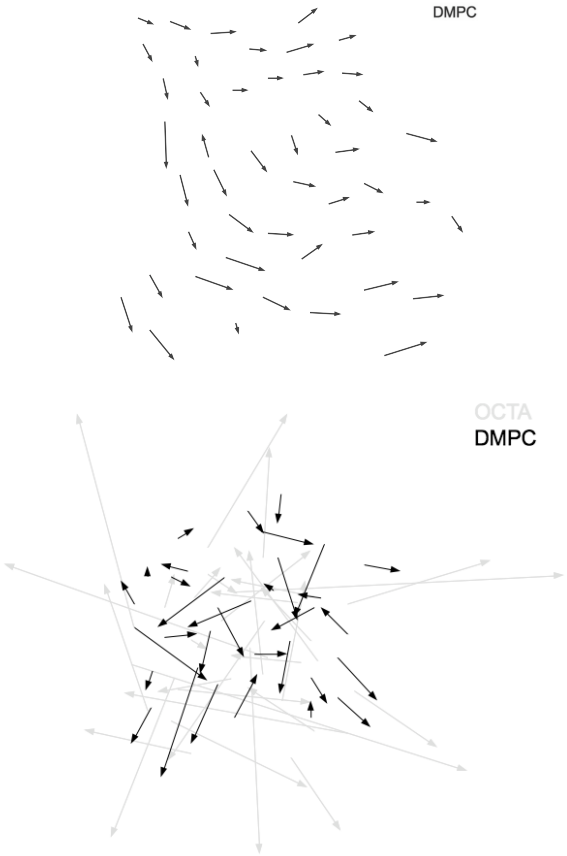

Figure 5: *Displacement for octanol and DMPC molecules Displacement for phospholipids in pure DMPC bilayer (top), and displacement for octanol and DMPC molecules in a bilayer in a temporal range of 4 ns (bottom).*

2) It is possible to extract diffusion coefficient D of lipid and alcohol by analizing msd. It is important to underline that we are interesting about in-plane molecular dynamics (dynamic along normal to bilayer is confined), so the space in wich molecules move can be considered as two-dimensional space. Msd values are calculated not over the whole 4 ns temporal range, but only for $t < 1$ ns, in order to have a good time average above all the range. From neutron scattering analisys [5] we know that diffusion coefficient for phospholipid and octanol are, respectively:

$$D_{phos} = 0.029 \mathring{A}^2/ps \quad (1)$$

$$D_{oct} = 0.035 \mathring{A}^2/ps \quad (2)$$

By MD simulation, it is possible to obtain mean square displacement through *subdiffusive relation*:

$$\langle \mathbf{r}^2 \rangle = 2dDt^c \quad (3)$$

where d is dimensionality of system and c the subdiffusive coefficient. By fitting through MD simulation data results:

$$D_{phos} = 0.0247 \mathring{A}^2/ps^c \quad (4)$$

where c=0.674

$$D_{oct} = 0.0354 \mathring{A}^2/ps^c \quad (5)$$

where c=0.756

As we can see, diffusion coefficient values calculated are very similar to experimental data (however it is important underline that the coefficient don't derive from identical models). Furthermore, if we compare DMPC diffusion coefficient in phospholipid-octanol bilayer with corresponding value for simple DMPC bilayer (D=0.012 $\mathring{A}^2/ps$ [1]) we can notice as octanol presence increases diffusional motion in membrane.

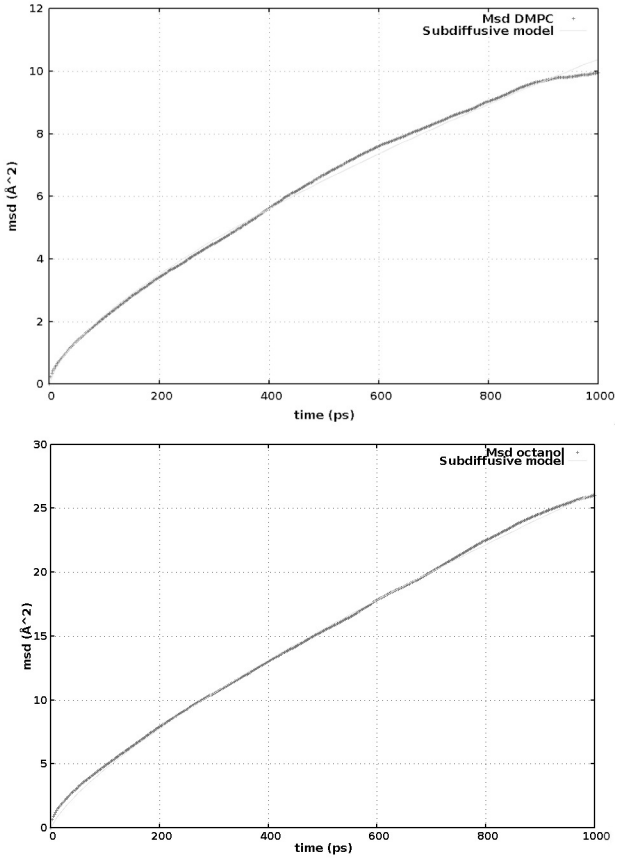

Figure 6: *In-plane msd for DMPC (up) and octanol (down) molecules. Crosses correspond to simulation data, lines to subdiffusive model fit.*

Conclusions

By analisys of MD trajectories of a bilayer composed by DMPC and octanol, we were able to understand how alcohol influences dynamics of bilayer. In particular we can say that:

-Octanol presence increases diffusion coefficient of phospholipid in bilayer, and subsequentially, membrane fluidity;

- By adding alcohol in bilayer, coordinative dynamics are no more visible. It is possible that this disruption influences formation and dynamics of lipid rafts in cellular membrane, and so all biochemical reactions that permits a regular cellular activity.

References

[1] Wanderlingh, U., D'Angelo, G. *et al.*: *Multicomponent modeling of quasielastic neutron scattering from phospholipid membranes*. Journal of Chemical Physics, **140**, 174901, 2014

[2] Staiti, M.: *Analisi di traiettorie MD e confronto con dati QENS da membrane biomimetiche*. Degree Thesis, 2012-2013

[3] Lee AG.: *Interactions between anesthetics and lipid mixtures. Normal alcohols.*. Biochemistry, **15 (11)**, 2448-2454, 1976

[4] S. A. Simon, T. J. McIntosh, M. L. Hines: *Molecular and cellular mech- anisms of anesthetics.*. S. H. Roth and K. W. Miller editors, Plenum New York, 279, 1986

[5] Finocchiaro D.: *Dynamical models of DMPC-octanol bilayers*. Activity report 2013, 21, 2013