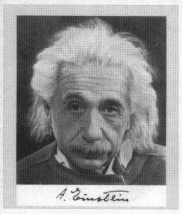
International Conference
"Functional Materials"
ICFM
2005
Crimea

International Conference "Functional Materials"

ICFM - 2005

ABSTRACTS



2005
World Year of Physics

Ukraine, Crimea, Partenit
2005

DQ-11/8 DIPOLAR CORRELATION FUNCTION AND MOLECULAR MOTIONS INTO FLUCTUATED POTENTIAL BARRER

M. Olszewski[1], A. V. Sapiga[2], N. A. Sergeev[1]

[1]*Institute of Physics, University of Szczecin, 70-451 Szczecin, Poland*
[2]*Faculty of Physics, Tavrida National University, 333007 Simferopol, Ukraine*

Many of NMR experimental values such as the second moment of NMR spectrum, spin-lattice relaxation rates, the time position and amplitude of the solid echo signals, and others are governed by the dipolar correlation function [1]:

$$h(t'',t') = w\sum_{i,j}\overline{a_{ij}(t'')a_{ij}(t')}, \tag{1}$$

where $a_{ij}(t)$ are the values, which describe dipolar interactions between nuclear magnetic moments.

The dipolar correlation function depends on the mechanism of the molecular mobility and its calculations are an important matter in researches of nuclear magnetic resonance in solids. The model of activated molecular motions over static potential barrier leads to the well-known Markov processes [2]. Molecular reorientations are often connected with the large structural fluctuations in solid dynamics. These fluctuations form additional internal degrees of freedom, which are not observed in NMR experiments and which lead to non-static potential barrier. The processes with time dependent potential barrier are the non-Markovian process of molecular mobility[3,4]. In the paper [5] we have shown that simple non-Markovian model of molecular mobility with fluctuations driven by bistable process of telegraphic type explains very well the observed temperature dependence of NMR spectra in natrolite crystal. In the present report we, using the stochastic master equation with random transition probability matrix in two-state model, obtained the following equation for the dipolar correlation function

$$h(t) = \overline{M}_2 + \left(M_2 - \overline{M}_2\right)\cdot e^{-2Wt}\cdot\left\langle \exp\left[2\int_0^t \widetilde{W}(\tau)d\tau\right]\right\rangle, \tag{2}$$

where $\overline{M}_2$ is the second moment of motionally narrowed NMR line and M_2 is the second moment of NMR spectrum in rigid lattice, $\widetilde{W}(t)$ is the fluctuated part of the transition rate W. In Eq.(2) $\langle\cdots\rangle$ denotes the average on the stochastic fluctuations of $\widetilde{W}(t)$. When $\widetilde{W}(t)\equiv 0$ (the fluctuations absent) we obtain the well known classical exponential decay of $h(t)$ [2]. We have calculated the dipolar correlation function $h(t)$ for some stochastic processes: Gauss-Markovian; Lorentz-Markovian and other ones [6]. The obtained results have been used for calculation of the temperature dependences of the second moment of NMR spectra, spin-lattice relaxation times ($T_1, T_{1\rho}$), the time position and amplitude of solid-echo signals.

1. P. Bilski, M. Olszewski, N. A. Sergeev and J. Wąsicki, Solid St. NMR **25** (2004) 15.
2. A. Abragam, The Principles of Nuclear Magnetism, Clarendon Press, Oxford 1961.
3. H. Sillescu, J. Chem. Phys., **104** (1996) 4877.
4. P.Hänggi, P.Talkner and M.Borkovec, Rev.Mod.Phys., **62** (1990) 251.
5. M. Olszewski, N. A. Sergeev and A. V. Sapiga, Z. Naturforsch., **59a** (2004) 501.
6. J.R.Klauder and P.W.Anderson, Phys.Rev., **125** (1962) 912.