Magnetic Resonance and Related Phenomena

Volume I

Proceedings

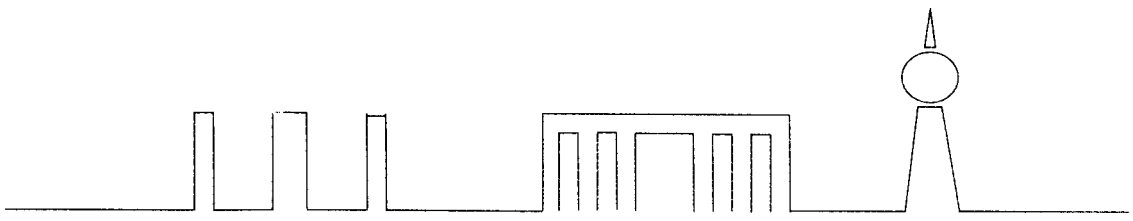
of the

Joint 29th AMPERE - 13th ISMAR

International Conference

Technische Universität Berlin

Berlin, August 2 - 7, 1998



Peculiarities of Quadrupolar Nuclei NMR Spectra Simulation into Non-Ideal Crystal Structures

H.M.Maksimova[1], N.A.Sergeev, A.V.Yatsenko[1]
University of Szczecin, 70-451, Szczecin, Poland
[1]Simferopol State University, 333036, Simferopol, Ukraine

Computer simulation of quadrupolar nuclei NMR spectra is very useful tool for intrinsic structural defects investigation into non-ideal structures and this method is, probably, the first approach to solids NMR imaging. It was been shown earlier [1,2] that the determination of total volume defects concentration is possible by using of the analysis of the angular dependence of the first moment of the NMR central transition line shape of quadrupolar nuclei. But this method is not useable for the separation of some possible kinds of irregular intrinsic defects into ionic crystals.

Into the case of small volume defects concentration it is possible to describe the situation as the "insulated" defects action, when the charged point defect presence lead to electric field gradient (EFG) tensor parameters distortion onto the nearest (≈1nm) nuclei. By the calculations of EFG tensor parameters for all possible positions of the picked kind of nuclei it is possible to obtain the array of the EFG tensor realizations. Taking into account the broadening of NMR line by direct dipole-dipole action and believe, that computed according to EFG tensor parameters frequency shift values are the expected values of Gauss distribution, the composition of this lines will be resulting simulated NMR spectrum. This method was used earlier for intrinsic defects investigation into ferroelectric $LiNbO_3$ congruently grown crystals [3]. But the volume concentration of intrinsic defects into congruent $LiNbO_3$ samples is relatively high and it is need to take into account the overlapping defects action to EFG tensor parameters onto pick kind of nuclei.

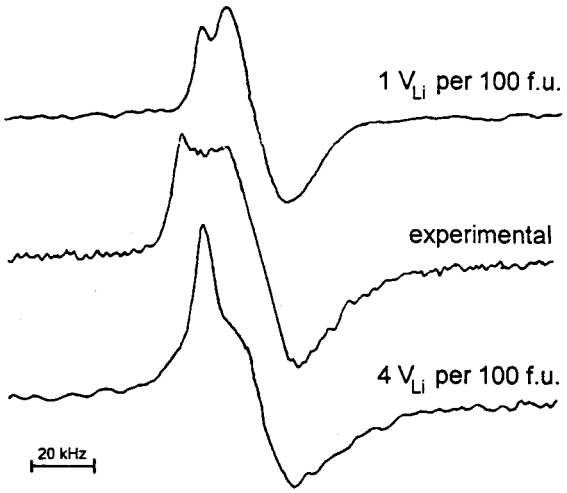
Thus the simulation of NMR spectra of ^{93}Nb nuclei into $LiNbO_3$ crystal can be fulfilled in such manner:

a) Taking into account the volume concentration of given type of defects this defects by a random way have been localized into the sphere with radius of 3 nm.

b) For each obtained a random defect configuration EFG tensor parameters have been calculated for all ^{93}Nb nuclei into the second sphere with radius of 2 nm and the center on Nb^{5+} ion (105 realization of EFG tensor in $LiNbO_3$ case). This procedure must be repeated - up to 200 ones - for another random defect sublattice configurations.

c) According to obtained EFG tensor parameters array the simulation of NMR spectra have been provided (taking into account the dipole-dipole broadening only) – as for central transition line, as for quadrupole satellites.

By this way it was simulated the angular dependencies of linewidth and the second moment of central transition line of ^{93}Nb NMR spectra as 1-st quadrupole satellites coupling and lineshapes for the seven different models [3] of probable defects of $LiNbO_3$ structure. The central line spectra at $\theta = 10^{\circ}$ (θ – the angle between $\mathbf{B}_0$ and **C**-axis of crystal) are showed in Figure (experimental one and simulated for two models). The additional narrow NMR line was identified as "free" Li ions vacancies (V_{Li}) action onto the nearest ^{93}Nb nuclei. By the comparing of the simulated and experimental data it was concluded that the most probable type of intrinsic defects in $LiNbO_3$ is the one [Nb_{Li}+3 V_{Li}] complex and "free" V_{Li} (in ratio 1:1 approximately) per 100 formula units. This result are in good agreement to as central line as satellites data. But this results are only preliminary because the influence of lattice distortion by defects can be relatively large.



[1] A.V.Yatsenko and H.M.Ivanova, Phys.of Solid State 37, 1237-1240 (1995)
[2] H.M.Ivanova, A.V.Yatsenko, and N.A.Sergeev, Sol.St.NMR 4, 381-385 (1995)
[3] A.V.Yatsenko, H.M.Ivanova, and N.A.Sergeev, Phys.B 240, 254-262 (1997)