

Control of the State of Intercalant in Layered Compound GaSe

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Abstract—A possibility of application of the nuclear magnetic resonance (NMR) method for estimation of spatial distribution of intercalated Li impurity in GaSe samples is considered.

Index Terms—layered semiconductors, intercalation, nuclear magnetic resonance

I. INTRODUCTION

The availability of two-dimensional atomic mobility of alkaline metals in the interlayer spaces of layered III-VI crystals enables to establish the content and uniformity of intercalant distribution by means of the NMR method. This possibility is based on a well-known principle of NMR tomography [1] when observation of a resonance from different parts of a sample performs in a gradient of magnetic field. From obtained information in a form of intensity distribution of resonance signal a pattern of a sample under investigations becomes formed. For biological objects as often as not a source of such information is NMR for hydrogen ¹H.

The idea of nuclear-magnetic tomography is sketched in Fig.1.

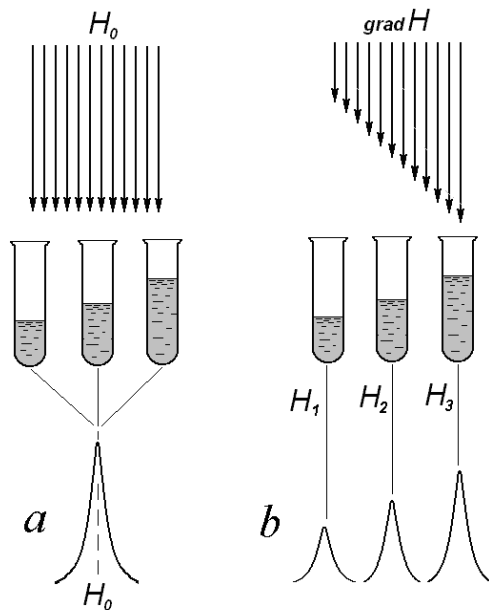


Figure 1. Sketch of NMR-tomography. Resonance spectra of three test-tubes filled with different amount of water placed in uniform (a) and gradient (b) magnetic fields

If test-tubes filled with different amount of water are placed in uniform magnetic field, the lines of each of them run into one resonance line which satisfies the condition

$$\omega = \gamma \cdot H_0,$$

where ω is the frequency of exciting radio-frequency field, γ is the gyromagnetic ratio for an investigated nucleus, and H_0 is the resonance field.

But at imposition of a scanning field having a gradient, there is a possibility to observe a spectrum of the separated lines which reflect the presence of test-tubes with different amount of the liquid.

II. EXPERIMENTAL

In our case the resonance was observed at nuclei of ⁷Li isotopes whose ions were intercalated into GaSe. NMR spectra at ⁷Li in Li⁺-intercalated GaSe samples were observed in a form of wide lines at a resonance frequency $f_0=13,495$ MHz by means of fast modulationless scanning magnetic field in the resonance range [2]. Quite high sensitivity of the spectrometer (10^{17} spin/cm³) was achieved because of the application of an induction-type spin-detector [3] and digital storage of spectra.

The samples being used for investigations had a rectangular form and dimensions of about 8×4×3 mm³. Each sample consists of a set of thin single crystal plates of gallium selenide intercalated with Li⁺ ions. For these samples in a uniform magnetic field there is a narrow NMR line of ⁷Li with a width of about 60÷80 mG.

To obtain a profile of the spatial distribution of Li⁺ ions, a linear gradient of the magnetic field at the GaSe samples was created by means of additional coils. A scheme of such an experiment is shown in Fig. 2. This gradient was directed along the crystallographic *c* axis, i.e. normally to the layers of GaSe.

At such orientation of the sample in the magnetic field because of the absence of diffusion of Li⁺ ions across the layers at infinitesimal width of the resonance a spectrum consisting of a set of separate NMR ⁷Li lines would be observed, each of which has its resonance field and, therefore, spatial coordinates of the layer. In the real spectrum the lines of the interlayer lithium are overlapped due to natural broadening mechanisms and an averaged profile of the intercalant distribution is registered.

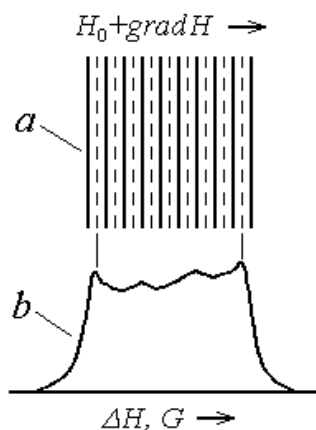


Figure 2. Scheme of receiving NMR ${}^7\text{Li}$ spectrum in intercalated GaSe at imposition of scanning magnetic field $H_0 + \text{grad}H$ to the sample: *a* – layered crystal, *b* – resonance spectrum of ${}^7\text{Li}$; solid lines - host atomic layers, dashed lines – Li^+ ions.

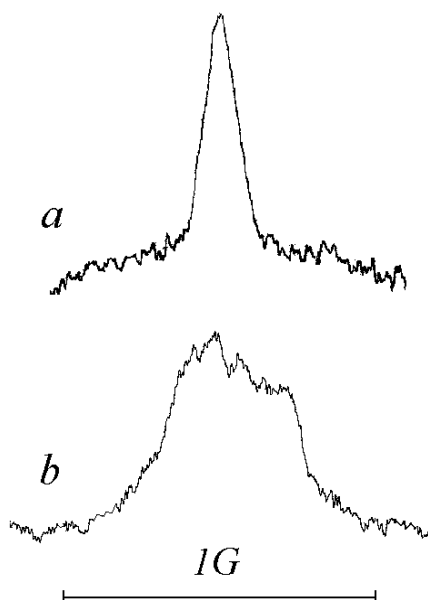


Figure 3. NMR ${}^7\text{Li}$ spectrum for intercalated GaSe in uniform magnetic field (a) and in the presence of magnetic field gradient (b) along the *c* axis. $\nu_0 = 13,495\text{MHz}$.

$T = 293\text{ K}$.

For weakening the influence of the immobile Li^+ ion phase on the spectrum of the mobile component the observation has been carried out in increased high-frequency field at the sample ($80 \div 100\text{ mG}$) when the wide resonance line becomes saturated and the narrow line intensity increases essentially.

In some cases at higher content of Li^+ ions it is possible to observe separate lines, resolved against others, what probably indicates on an excess of the intercalant in some ranges of the sample. Fig. 3 shows NMR ${}^7\text{Li}$ spectra for the Li -intercalated sample of GaSe located in uniform and gradient magnetic fields.

III. CONCLUSION

Observation of NMR ${}^7\text{Li}$ spectra in gradient magnetic field enables to receive information about distribution of lithium ions in a bulk sample of a layered compound GaSe.

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