Nuclear Magnetic Resonance Laboratory course Assignment 5

NMR on metals II: Liquid Gallium metal

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Abstract

Nuclear Magnetic Resonance (NMR) spectroscopy offers a unique window into the electronic and dynamic properties of materials, making it an invaluable tool for studying systems with complex atomic environments. Liquid metals, with their distinctive combination of metallic bonding and fluidity, present an intriguing subject for NMR investigation. Among these, liquid gallium is particularly noteworthy due to its unusual properties, such as a low melting point and high surface tension, which are coupled with metallic conductivity.

This laboratory experiment is centered on exploring the electronic and dynamic behavior of liquid gallium through NMR spectroscopy. Liquid gallium provides an excellent model for examining how atomic nuclei interact with conduction electrons in a liquid state, where atomic motion and electronic fluctuations are more pronounced compared to solid metals. By analyzing the NMR response of liquid gallium, particularly through the Knight shift and spin-lattice relaxation times (T1), we can gain insights into the local electronic environment and the influence of atomic dynamics on the NMR signal.

This experiment will take you through the process of measuring and interpreting the NMR spectra of liquid gallium, highlighting how its fluid nature impacts both electronic interactions and nuclear relaxation processes. The study of liquid gallium via NMR not only sheds light on the behavior of liquid metals but also deepens our understanding of the interplay between atomic motion and electronic structure in these unique materials.

1 Theoretical background

For these experiments, you will need the following theoretical background. Please prepare necessary mathematical expressions and derivations:

- Define the concept of the extreme narrowing limit in Nuclear Magnetic Resonance (NMR).
- Provide a qualitative explanation of the relaxation theory as introduced by Bloembergen, Pound, and Purcell.
- Analyze the phase diagram of metallic gallium, highlighting key transitions and phases.
- Summarize the nuclear spin characteristics of all NMR-active nuclei in metallic gallium.
- In liquid metallic systems, the spin-lattice relaxation time (T₁) typically results from a combination of electron-nuclear hyperfine interactions and the atomic motion of gallium atoms in the melt. Discuss the conditions under which these contributions can be distinguished and separated.
- Derive the equations for the electron-nuclear hyperfine contribution to the spin-lattice relaxation times for both nuclear spin systems, specifically $T_1^m(^{69,71}\text{Ga})$, and the quadrupolar interaction contribution due to the mobility of gallium atoms, expressed as $T_1^q(^{69,71}\text{Ga})$.
- How can we determine diffusion coefficients or viscosities from T_1^q in a liquid metal?

2 Tasks

Please work on the tasks step-by-step and summarize your observations thoroughly and logically when you hand in the assignment. Please provide data plots and calculations to underline your conclusions. We recommend the use of ONMR running in Origin7 or later, for data analysis.

- Utilize a pre-prepared coil containing metallic gallium as the sample.
- Calibrate and match the probes to encompass the resonance frequencies of both ⁶⁹Ga and ⁷¹Ga at the respective magnetic fields.
- Optimize digitization parameters for accurate signal acquisition.
- Acquire a high-quality spectrum for both nuclear spin sub-systems.
- Perform a measurement of the spin-lattice relaxation time (T₁) for both nuclei.
- Re-tune the system to the copper resonance frequencies and use the resulting signal for Knight shift determination.
- Plot the spectra of ⁶⁹Ga and ⁷¹Ga on a Knight shift scale, qualitatively analyze the linewidths, and correlate these observations with the known nuclear parameters.
- Plot and analyze the T₁ measurements for both isotopes.
- Conduct isotopic separation and calculate the electron-nuclear hyperfine contribution $T_1^m(^{69,71}\text{Ga})$ and the quadrupolar interaction contribution $T_1^q(^{69,71}\text{Ga})$.
- Estimate the viscosity for each spin subsystem using the quadrupolar relaxation times T_1^q ^{(69,71}Ga).

3 Literature

- 10.1103/PhysRev.73.679
- 10.1016/0022-3697(66)90043-6
- https://linkinghub.elsevier.com/retrieve/pii/S0066410317300327
- 10.1080/00018736700101425
- 10.1007/BF02422588
- 10.1016/0370-1573(77)90060-6