Thermal stabilization of neutron Larmor diffractometers

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Abstract. We report on the design of a support unit for the radio frequency (RF) coils of a Larmor diffractometer (LD) eliminating fluctuations of the Larmor phase resulting from thermal expansion of the support structures. The key component defining the spacing between the RF coils is a Zerodur bar with a very low thermal expansion coefficient ($\alpha = 7 \times 10^{-8}$ K$^{-1}$). This support unit will allow for LD measurements on the $10^{-6}$ accuracy level even if the ambient temperature is fluctuating.

1. Introduction

Neutron Larmor diffraction (LD) is a high resolution diffraction technique based on Larmor precession of neutron spins. One key property of LD is that the resolution is decoupled from the monochromatization and divergence of the neutron beam. At present, LD is available at TRISP at the FRM II and at FLEXX at HZB. At both instruments a resolution $\Delta d/d \sim 10^{-6}$ is achieved, further improvement by one order of magnitude seems feasible with an optimized design. Material properties measured by LD include the thermal expansion under pressure and at low temperature [1, 2], the spread of lattice spacing resulting from micro strains or structural phase transitions [3, 4], accurate absolute lattice parameters [5], and structural and magnetic domain sizes [6].

Rekveldt first pointed out the appropriate field geometry shown in Fig. 1 [7, 8]: A uniform DC magnetic field is placed up- and downstream the sample with boundaries oriented parallel to the diffracting lattice planes. The Larmor phase $\phi = \omega_L \times t$ accumulated by a neutron spin after passing both fields is proportional to the Larmor frequency $\omega_L = \gamma B_0$, with $\gamma = 2.916$ kHz/Gauss, and the time $t = 2L/v_\perp$ the neutron spends in the field, where the latter is given by the velocity component $v_\perp = \pi \hbar/(md_{hkl})$ perpendicular to the field boundary. Thus the Larmor phase $\phi = 2m/(\pi\hbar)\omega_L Ld_{hkl}$ only depends on the field integral $J_0 = 2\omega_L L$ and the lattice spacing $d_{hkl}$. Thermal expansion is measured by tracking the phase shift $\Delta \phi(T)/\phi = \Delta d_{hkl}/d_{hkl}$.

The Larmor diffractometers at FLEXX and TRISP use the resonance spin echo technique (NRSE). The PDs are formed by pairs of RF spin flippers $C_1 - C_2$ and $C_3 - C_4$ (Fig. 1), the surfaces of these flippers define the boundaries of the precession regions [9, 10]. Phase shifts are measured by scanning the RF flipper $C_4$ along the beam axis. The resolution is both limited by counting statistics and by instrumental phase instabilities $\Delta \phi_{\text{inst}}$, resulting from temporal fluctuations of the field integral $\Delta J_0$. $\Delta J_0$ arises from fluctuations of the frequency $\omega_{\text{RF}}$ applied to the spin flippers, or the spacing $L$ between the coils. The design target value is $\Delta J_0/J_0 < 10^{-6}$.
Figure 1. (left) Sketch of a Larmor diffractometer. An initially polarized neutron beam crosses the uniform field $B$ twice (polarizer and analyzer are not shown). The boundaries of $B$ are oriented parallel to the lattice planes $d_{hkl}$. In the resonance spin echo configuration (NRSE), instead of a uniform field $B$ four RF spin flippers $C_1 - C_4$ are used, and there is no field along the flight path between the flippers and in the sample region. (right) LD raw data measured at TRISP on germanium (220), $k = 1.92 \text{Å}^{-1}$, by scanning the position the RF flipper $C_4$ at two temperatures. The data points were taken at identical $\Delta L$ values and are vertically shifted by the phase shift. $\Delta \phi/\phi = \Delta d_{220}/d_{220} = 3.05(14) \times 10^{-5}$ induced by thermal expansion is consistent with $\alpha_{\text{Ge}} = 6 \times 10^{-6} \text{K}^{-1}$. for the existing LDs and $10^{-7}$ for next generation instruments. $\omega_{\text{RF}}$ can easily be stabilized to the level $10^{-8}$ by using stable reference oscillators, such as oven controlled quartz or rubidium clocks.

The main source of instability is then the linear thermal expansion of the structures carrying the coils, an aluminum profile in the case of TRISP and FLEXX. The thermal expansion of the Al with a coefficient $\alpha_{\text{Al}} = 2.31 \times 10^{-5} \text{K}^{-1}$ directly affects the field integral and thus the phase, such that $\Delta \phi/\phi = \alpha_{\text{Al}} \times \Delta T$. At TRISP in the experimental hall of the FRM II, the ambient temperature is very stable and drifts typically less that 0.1 K within 12 h, corresponding to $\Delta \phi/\phi < 2.3 \times 10^{-6}$. Only if the temperature drift is slow ($< 0.2 \text{K/h}$), the whole support structure is thermalized and the phase drift can be corrected by measuring the ambient temperature. Faster temperature drifts make measurements beyond the $10^{-5}$ level impossible. Besides this large linear thermal expansion of the support structures, there are certainly additional thermal drift mechanisms acting on the effective coil spacing $L$ and thus on the Larmor phase, including bending of the support structure and bending of the DC coil wires, which leads to a curved coil surfaces and eventually to an effective shift of the coil center. These mechanisms are probably smaller than the linear expansion effect. Fluctuations of the DC current $I_0$ enter only in second order as $\delta \phi \sim (\delta I_0/I_0)^2$. With stabilized power supplies $\delta I_0/I_0 \sim 10^{-4}$, and $\delta \phi \sim 10^{-8}$ can be neglected. However, if there is as asymmetry in the RF flippers, resulting, for example, from an offset between the centers of the RF and DC coils along the beam path, current fluctuations might also enter the phase in first order and could become significant.

There are several strategies to minimize these drifts: (i) Exact measurement of the spacings $C_1 - C_2$ and $C_3 - C_4$, for example by a laser interferometer, and active compensation of the drift. As the coils are sitting on rotation units, it is difficult to find adequate points for attaching reference mirrors. (ii) Constructing the support with low thermal expansion materials. As the support must be non-magnetic to avoid stray fields disturbing the Larmor phase, Invar ($\alpha = 1.5 \times 10^{-6} \text{K}^{-1}$) is not usable. Granite can be machined and is used for constructing precise and stable structures and tables, but the thermal expansion is too large for our application.
The Zerodur ceramic (Schott) shows excellent stability, the type 0 material has a very low \( \alpha = 0 \pm 2 \times 10^{-8} \text{K}^{-1} \). The construction of large structures from Zerodur is possible, but in the present case precluded by the high prize. We thus decided to keep the supporting aluminum structure and to compensate the linear expansion of the support by defining the spacing between the coils by a thin Zerodur bar.

**Figure 2.** Support unit for RF coils \( C_1 - C_2 \) or \( C_4 - C_3 \).

**Figure 3.** Longitudinal cut through the unit (side view). The center of the base plate (1) defines the reference point. The carriage (2) with motor drive and optical linear encoder allows for translational scanning of one RF coil. The post (3) is attached to the base plate with the pivot pin (4) to provide a suspension point (reference point) for the Zerodur bar (5). The right unit includes a base plate (6), and a carriage (7) suspended with linear bearings on (6). The post (9) is connected to (7) via the pivot pin (6). The spring (10) with setscrew (11) presses (7) against the Zerodur bar (5).

The design is shown in Figs. 2 and 3. The key component is the Zerodur bar (20 × 20 × 500 mm\(^3\)) keeping the distance between the centers of the base plate of the left unit and the upper part of the right unit constant. The end faces of the bar rest on flat posts being attached to pivot pins in the left bottom and right upper plates. The latter is suspended on a precise linear bearing (Schneeberger R6-250) and is pressed against the Zerodur bar by a spring (60 N). Thus the right carriage can translate with respect to the base to compensate thermal expansion of the aluminum support structure (not shown). An additional motor driven translation stage incorporated in the left unit is used to scan the spacing between the coils to measure the spin echo phase as shown in Fig. 1 (right). The pitch and yaw angles over the translation range of ±25 mm are < 70 \( \mu \text{rad} \) and < 20 \( \mu \text{rad} \), respectively. Over short translation distances, both angles
Figure 4. Left translation unit: (1) Aluminum base plate. (2) Linear ball bearing (Schneeberger R6-250) (3) Ball screw (Hipp KGT-F-08-01-132-74-O-IT1, slope 1 mm, dynamic load 850 N, material 1.1213 Cf53, $\alpha = 11.5 \times 10^{-6}$/K. (4) Fixed bearing. (6,7) Stepping motor Phytron ZSS 25.200.0.6 with HarmonicDrive gear HD 05/80. Linear encoder Heidenhain LIP 481, precision $< 0.15 \mu$m (not shown).

The phase are $< 10 \mu$rad. Special care was taken to avoid drifts in this translation by thermal expansion of the drive screw (Fig. 4). First, the position is measured by a precise linear encoder (Heidenhain LIP 481, error $< 0.15 \mu$m) directly attached to the translation unit, thus that thermal expansion of the ball screw (Fig. 4, (3)) is directly monitored. Second, the expansion of the screw is compensated by an asymmetric mount to the carriage, thus that expansion of the screw and of the carriage compensate.

Figure 5. Phase shift vs. total counts (eq. 1) for $\Delta L = 0.5$ mm, $(\lambda = 4 \AA$, $\omega_{RF} = 2\pi \times 500$ kHz), $P = 0.5$.

In summary, we designed a support for the RF flippers of a LD with passive compensation of the linear thermal expansion by using a Zerodur standard. The unit is easy to manufacture in institute workshops and eliminates the dominating phase instability resulting from thermal expansion of support structures. We tested the stability by repeated measurements of the Larmor phase on the aforementioned Ge (220) Bragg reflection. On a time interval of 12 h, the phase shows random fluctuations in the order of $\Delta \phi/\phi \sim 1 \times 10^{-6}$, corresponding to an effective variation $\delta L \sim 1 \mu$m of the total length $L = 1$ m, where the accuracy was not limited by counting statistics. Operation on a $10^{-6}$ accuracy level will thus be possible in experimental facilities with fluctuating ambient temperature.
For the design of future Larmor diffractometers with relative accuracies around $10^{-7}$, first the aforementioned additional drift mechanisms resulting from bending of the support and heating of the coils have to be quantified and reduced. If we assume, that these drifts are independent of the spacing of the coils, the resolution can be increased by a factor 4 using the present coil and support design by increasing the coil spacing from presently 0.5 m to 2 m. Further the frequency applied to the coils can be increased. Presently we operate the coils at the relatively low frequency of 200 kHz to avoid heating. The temperature in the center of the beam window, where cooling of the coil is worst, rises only by 3 K after switching the coil on. Increasing the frequency by a factor 2.5 to 500 kHz will induce additional thermal drifts, and probably will require a modified coil design with reduced bending of the wires.

Finally we briefly discuss counting statistics. The statistical accuracy is estimated via the derivative of the cosine-shaped signal in eq. 1. The phase error $\delta \Delta L$ is

$$\delta \Delta L = \Delta L_{\text{period}} / (\pi P \sqrt{2I_{\text{total}}})$$

(1)

where $\Delta L_{\text{period}}$ is the period of the cosine, $P$ is the polarization and $I_{\text{total}}$ the total number of counts (the sum of all data points). Eq. 1 is shown in Fig. 5 for typical parameters. An error $\delta \Delta L < 0.4 \mu m$ is required for the resolution $10^{-7}$, which is obtained for $I_{\text{total}} > 3 \times 10^5$. There is the question on how many signal periods should the total counts be distributed? The number of signal periods has an influence if the period $\Delta L_{\text{period}}$ is not a fixed parameter in the fit and if the phase shift is far from $\Delta L = 0$, which happens usually when the phase travels due to thermal expansion of the lattice $d_{hkl}$. In this case the phase error $\delta \Delta L$ is also affected by the error in $\Delta L_{\text{period}}$. The latter is minimized by increasing the number of signal periods. At TRISP, it turned out as a good compromise to use 4 signal periods, which fit in the limited translation range of $\Delta L$ even for the shortest wavelengths.

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