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Thermo-elastic frequency domain analyses for a cryogenic temperature controlled precision sample holder

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Abstract
When designing a sample manipulator for use in synchrotron beam lines at temperatures as low as 4 K, the significant decrease in specific heat capacity and increase in thermal diffusivity of solid materials poses unique challenges for temperature control. In this particular application, electrical noise from the thermal control system is causing significant temperature fluctuations in the components due to the strongly reduced heat capacity at low temperatures. Due to increased thermal diffusivity at low temperatures, these temperature fluctuations are transferred to the sample location up to relatively high frequencies, resulting in thermo-elastic deformation dominating the overall position stability budget of the experiment carried out in the beamline. This article shows how the magnitude of this drift resulting from the control noise is predicted using a thermo-elastic frequency domain model, created from the output of a commercial finite element package. This model is used for a frequency domain analysis of the drift rate, which is then used to propose design steps to reduce the effect of the control noise on the sample drift rate.

Thermal control, frequency domain modelling, cryogenics, finite element modelling

1. Introduction and system overview

MI-Partners was involved in the design of a sample manipulator for use in high vacuum and at cryogenic temperatures. The manipulator needs to position a sample at the desired location, and thermally condition this sample at a constant temperature. The sample temperature is to be set in the range of 4 K to 293 K. These kind of manipulators are used in beam lines of synchrotron radiation facilities, for example for crystallography. For confidentially reasons, the system has been abstracted and result values have been scaled.

A simplified overview of the system is shown in Figure 1. The thermal conditioning is performed by having access to a cold source with a temperature below the desired sample temperature. This cold source is connected to a copper bar through a pre-defined thermal resistance (R). The copper bar is connected to the sample support by a braid.

The cold source, for example a pulse tube cryocooler, exhibits slow temperature fluctuations which exceed the stability requirements for this system. Therefore, a temperature control system is required to suppress the disturbance of the temperature variation of the cold source.

A feedback controller uses a sensor to measure the temperature at the copper bar and applies power through a heater to keep the copper bar thermally stable at the desired temperature. By these means, the sample is also kept at a stable temperature.

There are two main performance criteria for this subsystem:

- The absolute temperature at the sample position
- The position stability of the sample (drift rate)

The temperature requirement is related to the type of research: For example, material characterization at a certain temperature. The requirements on temperature accuracy are not that strict and can be achieved by calibrating the thermal control system using an external temperature sensor at the sample location. This is possible due to the highly reproducible nature of the system.

The position stability requirement is related to the imaging quality: position drift leads to blurring. As the duration of the experiment is not very long (typically tenths of a second to one minute), the position stability is specified as drift rate velocity, which should remain well below a nanometer per minute.

During imaging, there are no active components (including the manipulator) except for the thermal feedback controller. Direct feedback based on the actual sample position is not possible, so the drift rate is kept low by keeping the temperature constant.

This article investigates one of the issues encountered during the design of this thermal control system, with the thermo-elastic deformation of the sample support as the prime performance parameter. In section 2, the expected issues are described. In section 3, the modelling and analyses to quantify the issue are shown. The simulation results are shown in section 4, with proposed design improvements in section 5. The summary and conclusion are given in section 6.

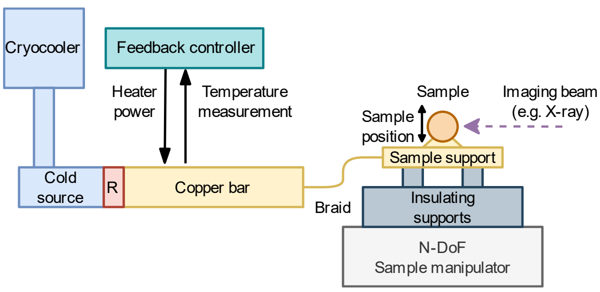

Figure 1. System overview.

2. Thermal time constants at cryogenic temperatures

The connection between the cold source and the sample consists mostly of OFHC copper. A high conductivity for the copper parts is desired such that the sample can reach a temperature close to that of the cold source, in the presence of disturbance heat fluxes from the sample manipulator. The lowest achievable temperature at the sample position is an additional performance figure for this system.

When cooling a copper part down from room temperature to cryogenic temperatures of 4 K, the material properties change as shown in Table 1. The thermal conductivity of the copper parts increases (factor 2.4) and the specific heat capacity decreases (factor 3850). What follows is a strongly increased thermal diffusivity (factor 9260) at cryogenic temperatures. The thermal time constants of the system are inversely proportional to the thermal diffusivity: the thermal system dynamics become fast. For example: a copper part with a first thermal time constant of 1000 s at room temperature would have a time constant of approximately 0.1 s at 4 K, which means it reacts fast and can follow high frequency disturbances.

Table 1. Thermal conductivity, specific heat capacity and thermal diffusivity of OFHC C10100 copper RRR150 [1].

Temperature [K]	C_P [J/kg/K]	k [W/m/K]	$\frac{k}{\rho \cdot C_P} \propto 1/\tau$
293	385	400	1.16e-4
77	196	557	3.16e-4
15	3.0	3038	1.12e-1
4	0.1	962	1.07

2.1. The issue: Thermo-elastic sample drift due to control noise

As mentioned earlier, the system contains a thermal feedback controller. This control system also has broadband temperature sensor and heater amplifier noise, which manifest as noise on the power output of the controlled heater.

The magnitude of this noise is small, but on the small thermal capacitance of the copper bar this already causes significant temperature fluctuations. Due to the small time constants of the system, these temperature fluctuations are transferred to the copper sample holder up to relatively high frequencies.

The temperature fluctuations in the sample holder cause thermo-elastic deformation: the deformation is small, but due to the relatively high frequencies, the control system is the dominant contributor to the overall drift rate.

2.2. Approach to quantify the thermo-elastic drift

A first estimate based on lumped capacitance modelling and noise specifications has shown the occurrence of thermo-elastic drift due to control loop noise. A more detailed analysis needs to be performed to quantify this effect more accurately, such that the proper design choices can be made in order to reach the drift rate requirements.

The following approach is used: firstly, the power spectral density of each noise source is measured. Secondly, a thermo-elastic finite element model is created that provides the frequency domain input-output relation at the points of interests: input is heater power, outputs are temperature at the control sensor and position at the sample. Based on the conductivity and capacitance matrices from the finite element simulation, a reduced order state-space model is created in Matlab. Thirdly, this state-space model is used in Matlab for simulations. This simulation involves the closing of the thermal control loop from temperature sensor to controlled heater and the application of disturbances. Finally, the expected sample drift rate is quantified for the modelled disturbances and if needed, design steps are proposed to improve the behaviour.

The approach shown above is commonly applied [2] when it comes to analysing mechanical or electrical dynamics, and finite element packages support such analyses. In the finite element software package used at MI-Partners (Ansys), thermo-elastic frequency domain analyses or the use of broadband heat flux inputs in transient thermal analyses are not standard functionality. However, MI-Partners has custom tooling to obtain reduced order frequency domain models based on a Krylov basis [4], from the conductivity and capacitance matrices generated by Ansys.

3. Disturbance quantification, thermo-elastic modelling and performance evaluation

This section shows the modelling of the system in order to evaluate the effects of disturbances, using the steps described in the previous section.

3.1. Quantification of control system noise

A commercially available temperature controller is used in this system, selected based on its low noise specifications for both sensor noise and heater amplifier noise. The periodogram of both noise sources has been quantified as shown in Figure 2 and Figure 3. Together these noise sources are referred to as 'control system noise' in this article. The measurements also contain some low frequency drift.

The noise in these figures is shown in power spectral density (PSD) format [3], which gives the noise power per Hz as a function of frequency for both sensor temperature and heater power. Noise components with frequencies much lower or higher than the measured frequency range do not contribute much to the total sample drift rate. The former (<< 1 mHz) due to the fact that the specification is on drift rate [nm/s] instead of position accuracy [nm]. The latter (>> 1 Hz) due to the limited bandwidth of the feedback controller and the time constants of the controlled thermal system.

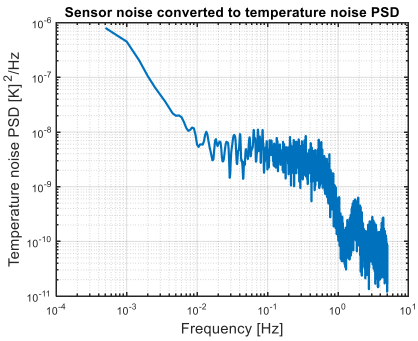

Figure 2. Measured sensor noise, converted to temperature noise PSD using resistance and sensitivity at cryogenic temperature.

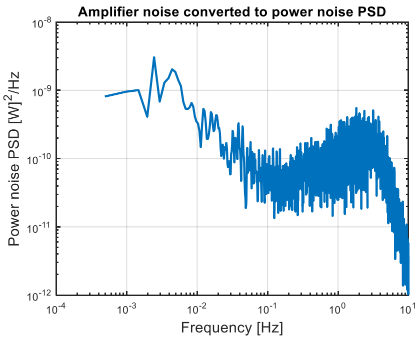

Figure 3. Measured amplifier noise, converted to heater power PSD at peak amplifier power.

3.2. Dynamic thermo-elastic modelling

A dynamic thermo-elastic model is required to evaluate the sample drift rate due to control noise shown in the previous section. Due to geometrical complexity, it was decided to create a finite element model based on a CAD model of the system. The creation of the dynamic thermo-elastic model follows the basic structure of a thermo-elastic model in Ansys: a transient thermal analysis followed by a static structural analysis.

Because the physical parameters such as the thermal conductivity, specific heat capacity, coefficient of thermal expansion and Young's modulus are strongly temperature dependent, the frequency domain model is linearized around a certain operating temperature.

As such, a steady state thermal analysis with temperature dependent parameters is performed first to determine the temperature of each component, which determines the value of the constant physical parameters for the dynamic analysis. During operation of the device, there is little temperature variation and as such the physical parameters can be assumed constant around that operating temperature.

The outputs from the Ansys transient thermal analysis are the thermal conductivity and thermal capacitance matrices, and the nodal input and output vectors. A model reduction step is performed on these matrices to obtain a more compact model.

3.3 Model order reduction and elastic deformation

Tooling is available at MI-Partners for model reduction using a modal basis or a Krylov basis [4]. Initially, a modal (eigenvalue) model reduction was chosen for the reason that this reduction method is very close to existing Ansys functionality for mechanical dynamics: it requires the calculation of the eigenvectors and eigenvalues, with residual vectors to correct for mismatches in static conductivity. For this thermal model of a cryogenic system however, the difference in time constants between slow modes (e.g. warm insulator parts) and fast modes (e.g. cryogenic copper parts) can become very large compared to a typical mechanical dynamics analysis. This large difference originates from the low capacitance of the cryogenic parts. This means that a large amount of modes would be required in order to properly capture the relevant input-output behaviour. Not doing this would result in a modal model that mostly contains the slow internal modes of the insulating parts. Alternatively, sub-structuring could be used to overcome this problem.

A Krylov basis [4] was used for model reduction. This reduction method required neither a large amount of shapes nor an a-priori model reduction in Ansys. A comparison between the reduced order and full order model is shown in Figure 4.

The final step is to use the thermal shapes as input in a Ansys static structural analysis to calculate the displacement shapes and obtain the thermo-elastic dynamic model.

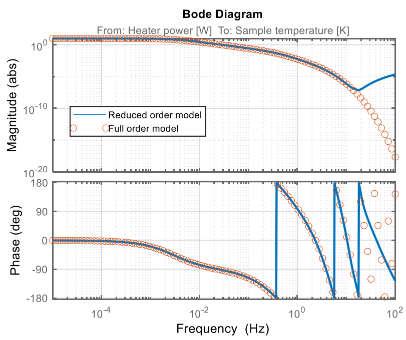

Figure 4. Reduced order model (blue), with full order model (red).

The model order reduction was performed before transforming the output from temperature to displacements. As the mechanical parameters of the critical parts are very similar (mostly copper), the Krylov shapes that represent the dominant thermal behaviour also represent the dominant displacements. This has been verified with a higher order model.

3.4 Performance simulation of controlled system

Once a thermo-elastic state-space model has been obtained, it needs to be evaluated by placing it in a feedback control loop. The feedback controller is tuned with the following trade-off in mind: it needs to have sufficiently high bandwidth to deal with the slowly varying temperature of the cold source (its primary function) and reject heater amplifier noise and heat flux inleaks, while the bandwidth should be sufficiently low to reduce amplification of temperature sensor noise.

For analysing the noise effects, a frequency domain Dynamic Error Budgeting analysis [2] is a useful method. For non-stationary deterministic disturbances such as the slowly varying cold source temperature, a time domain error budgeting analysis is more convenient.

The feedback control loop is shown in Figure 5, which is implemented in Matlab Simulink. This can be used for frequency and time domain analyses.

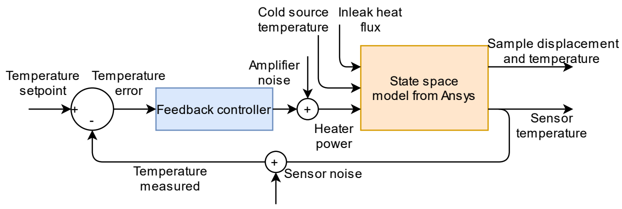

Figure 5. Example of thermal control loop in Matlab Simulink.

4. Performance results

First, a time domain simulation of the effects is shown using the time domain data behind Figure 2 and Figure 3. The time domain simulation has the advantage that it can include deterministic, non-stationary disturbances. The frequency domain analysis that follows after will give insight into the relevant aspects of the stochastic disturbances.

A detailed analysis of each disturbance source is outside the scope of this article, the focus will be on the effect of the control noise. In this case the time domain measurements of the sensor and amplifier noise are used as input for the closed loop system show in Figure 5. In Figure 6, the resulting closed-loop temperature fluctuation at the control sensor is shown in blue, and the temperature fluctuation at the sample in red. Due to the small thermal time constants of the system, the attenuation of temperature fluctuations between the temperature sensor and the sample support is very limited. The resulting thermo-elastic deformation at the sample holder is shown in Figure 7, which closely follows the temperature fluctuation of the sample support. The sample displacement is dominated by the thermo-elastic displacement of the thermally conductive parts of the sample support (Figure 1). Investigating the displacement at multiple points in the sample manipulator shows that the temperature fluctuations barely affect the insulating parts and the components behind it. From the thermo-elastic displacement, the drift velocity in the relevant time frame (tenths of a second to a minute) can be calculated.

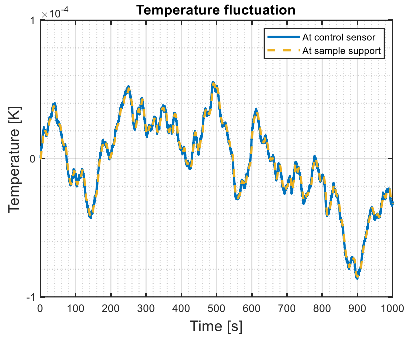

Figure 6. Temperature fluctuation at the control sensor and at the sample, showing almost no attenuation.

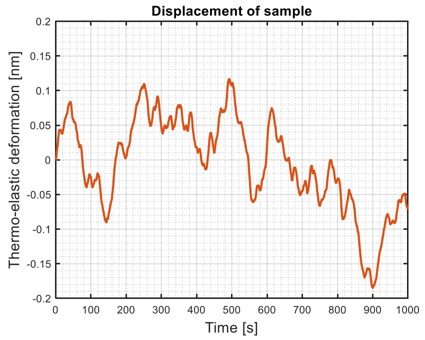

Figure 7. Displacement at the sample over time.

The analysis can also be performed in the frequency domain by using the measured PSD from Figure 2 and Figure 3 as input for the closed loop system from Figure 5. The output is a PSD of the sample velocity due to control system noise. This approach follows the standard dynamic error budgeting framework [2]. This frequency domain analysis gives additional insight into which noise frequency ranges are relevant for performance. This is valuable information in case a design change needs to occur to increase the system performance.

The effect of sensor and amplifier noise on the closed loop system is shown in Figure 8, in the form of a cumulative power spectrum (CPS) of the sample velocity. A CPS shows the cumulative contribution of each frequency component, and can be obtained by integrating the PSD over frequency. This is effectively a sum-of-squares of each frequency component. This shows that the low-frequency (< 1 mHz) drift of the sensor and amplifier, which seemed dominant over high frequencies in Figure 2 and Figure 3, becomes insignificant when looking at the velocity of the controlled system. The noise in the frequency range between 1 mHz and 2 Hz results in the greatest velocity disturbance at the sample position. Adding the two contributors leads to approximately 0.47 nm per minute (3σ value), which is close to the drift rate budget for this particular disturbance.

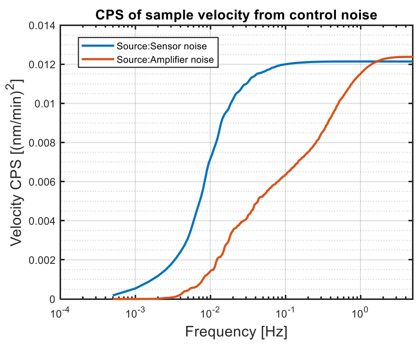

Figure 8. Cumulative power spectrum of sample velocity due to amplifier and sensor noise.

5. Mitigating the effects of control loop noise

Design changes had to be implemented to reduce the impact of this disturbance. Four paths were considered, which are discussed in this section: reducing the source noise magnitude, reducing sample holder sensitivity, increasing time constants by increased thermal resistance and decreasing temperature fluctuation by increased thermal capacitance near the heater. The frequency domain analysis gives insight into which measures make sense to reduce the dominant components.

The control system is already state-of-the-art in terms of signal to noise performance for commercially available hardware. Further improvement would likely require custom electronics development, possibly with marginal improvements on quality. The bandwidth of the control system has already been optimized to balance the different disturbances in the system.

Reducing the sensitivity for temperature fluctuations at the sample support would require substantial design changes in that module, which was not desired.

Adding a thermal resistance within the copper bar capacitance between heater and sample would reduce the noise transfer by decreasing thermal diffusivity, but would lead to greater temperature difference between cold source and sample.

Increasing thermal capacitance near the heater resulted in a feasible solution as the drift rate was already close to the target.

6. Summary, conclusion, future work

For a sample manipulator as shown in this article, noise disturbance from thermal control electronics can often be assumed negligible at room temperature and for cryogenic temperatures as low as (and somewhat below) the boiling point of liquid nitrogen. This is due to the high heat capacity and low thermal diffusivity of the components.

At liquid helium boiling temperatures (~4.2 K) however, the thermal time constants of copper components decrease by almost four orders of magnitude. Combined with tight position drift specifications, this results in a situation where electrical noise from the control loop is a relevant source of thermo-elastic disturbance for the cryogenic precision manipulator.

By measuring the disturbances, creating a frequency domain thermo-elastic model and evaluating the resulting thermo-elastic drift, this effect can be quantified and mitigation steps can be taken during design.

The thermo-elastic model can be created by using a commercial Ansys finite element package, but requires custom tooling in postprocessing to obtain a reduced order frequency domain model. For future work remains the measurement of the thermo-elastic drift rate on the actual realized system.

References

[1] Simon N J, Drexler E S and Reed R P 1992 Properties of Copper and Copper Alloys at Cryogenic Temperature, p7-16 and p7-1

[2] van Eijk J, Jabben L, Hobbelen D G E and Spronck J W 2004 Dynamic Error Budgeting, a Tool for Designing High Precision Devices *Control of precision systems: ASPE 2004 spring topical meeting* p97-97

[3] Oppenheim A V, Willsky A S and Young I T 1983 *Signals and systems*. (Prentice-Hall, Englewood Cliffs, New Jersey)

[4] Aarden W, Bukkems B, Limpens M and Ruijl T 2020 Applied thermo-elastic model reduction *Euspen Thermal Issues Proceedings 2020.71-74*