Thermally induced deformations in electron microscopy

CHALLENGES AND OPPORTUNITIES FOR SYSTEM IDENTIFICATION

Thermal effects are becoming increasingly important in efforts to enhance the performance of electron microscopes. Therefore, accurate thermal-mechanical models are desired for analysis and control. Modelling thermal systems from experimental data, i.e. system identification, is challenging due to large transients, large time scales, excitation signal limitations, large environmental disturbances, and nonlinear behaviour. An identification framework has been developed to address these issues. The presented approach facilitates the implementation of advanced control techniques and error compensation strategies by providing high-fidelity models.

ENZO EVERS, RONALD LAMERS AND TOM OOMEN

Introduction

Thermo Fisher is a leading manufacturer of electron microscopes. Their high-end (transmission) electron microscopes are developed and produced in Eindhoven (NL). These systems are capable of visualising objects at the atomic scale with a resolution down to 50 picometer (sub-Ångström resolutions).

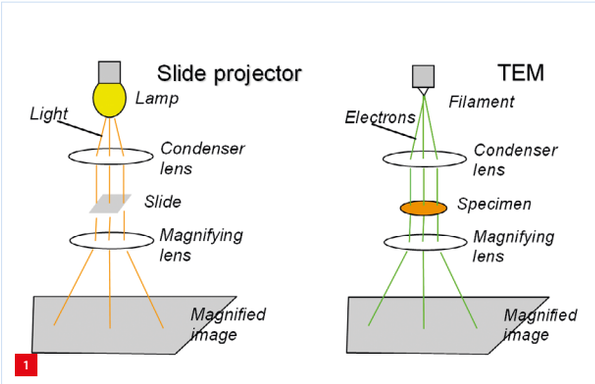
The goal of an electron microscope is to acquire high-quality and high-resolution images of a specimen. The basic operation principle of an electron microscope, which is similar to that of a conventional light microscope or slide projector, is shown in Figure 1. Whereas a slide projector works with light and optical lenses, an electron microscope works with electrons and electromagnetic lenses.

A general overview of a transmission electron microscope is shown in Figure 2. The electron beam is generated inside the electron source, and the electrons pass through the condenser lens system, which makes the electron beam parallel. Then, the electron beam passes through a thin specimen that is mounted on a sample manipulation stage. This stage can move the specimen with respect to the electron beam, hence a large area of the specimen can be imaged. The corrector lens system is an additional module that can be placed on the electron microscope to correct for optical aberrations. Finally, the projector lens system magnifies the image and projects it onto a camera.

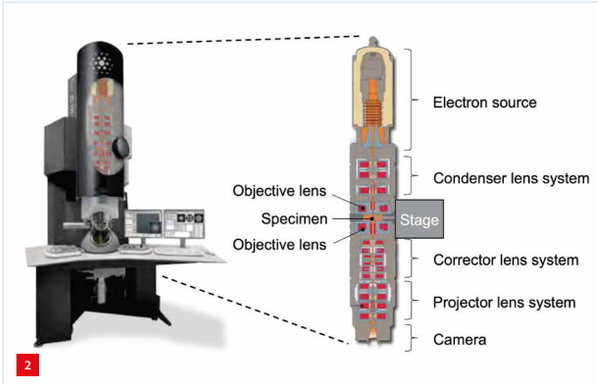
AUTHORS' NOTE

Enzo Evers (Ph.D. candidate) and Tom Oomen (associate professor) are both associated with the Control Systems Technology group within the department of Mechanical Engineering at Eindhoven University of Technology in Eindhoven (NL). Ronald Lamers works as a thermal dynamic design engineer at Thermo Fisher in Eindhoven.
The authors gratefully acknowledge Niels van Tuijl for his contribution to this work.

e.evers@tue.nl
www.tue.nl/cst
www.thermofisher.com
www.toomen.eu



Similar operation principle of a slide projector and a transmission electron microscope (TEM) [1].



General overview of a transmission electron microscope [2].

Advanced Thermal Control Consortium

Thermo Fisher has joined the Advanced Thermal Control Consortium. The aim of this consortium is to advance the theoretical and applied approaches to design, simulation, measurement and compensation techniques essential for the development of precision modules/systems subject to internal or external thermal loads [3]. Within this consortium, a fruitful collaboration between Thermo Fisher and Eindhoven University of Technology has been set-up to expand the identification and control approaches available for thermal-mechanical systems.

ADVANCED THERMAL CONTROL CONSORTIUM

WWW.TUE.NL/HTSC

Because an electron microscope is capable of visualising objects at the atomic scale, it is a key enabler for nanotechnology, life science, material science and semiconductor technology. Electron microscopes are increasingly being used as analysis tools in laboratories and industry. Whereas the material science market is pushing the boundaries with respect to resolution of electron microscopes, markets as semiconductors and life science are pushing the boundaries with respect to throughput. In view of these increasing demands for throughput and resolution, the stability of electron microscopes becomes increasingly important.

Stability

Acquiring high-resolution images requires the exposure time of the camera to be sufficient long. The image acquisition process takes time, because a sufficient amount of electrons need to be detected in order to provide enough contrast in an image, which is the main measure for image quality. In fact, the contrast improves with increased exposure time. During the exposure time, the specimen must remain stationary with respect to the electron beam. Movement of the specimen, known as drift, would lead to a blurred image, as shown in Figure 3. In this context, stability is defined as minimal drift of the sample position with respect to the electron beam. At present, the state-of-the-art approach is to wait (minutes to hours) until the drift is low enough for high-quality imaging, which significantly reduces the throughput of the system.

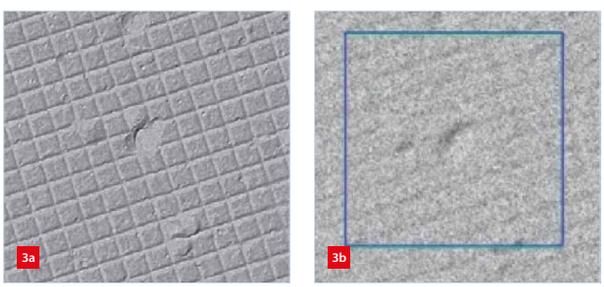


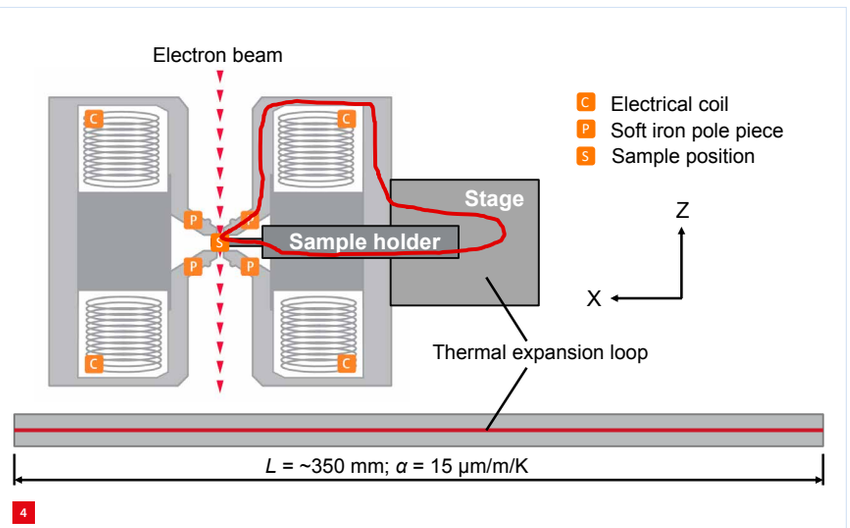
Image of an object (gold) [4].
(a) In high contrast.
(b) With blur.

For example, in life science applications a so-called single-particle analysis is performed to study single proteins that perform key roles in diseases in their native context in the cell at near atomic resolution. In such analyses, the microscope can be taking images automatically for several days, during which image quality, and thus stability (< 10 nm/min) of the electron microscope must be guaranteed.

Sensitivity

In Figure 4, a more detailed view is given on the specimen location inside the electron microscope. The specimen is placed on a sample holder, which will be positioned inside the sample manipulation stage and the electron microscope. Also shown in Figure 4 is the thermal expansion loop.

The thermal expansion loop covers parts of the electron microscope on which the stage has been mounted, parts of the stage, and parts of the sample holder. If the temperature of these parts changes due to thermal disturbances, they will deform, which will cause drift of the sample position with respect to the electron beam. The thermally induced deformation in X-direction is far more dominant than in Z- and Y-direction, therefore the thermal expansion loop can be considered as a sum of 1D expansions in X-direction of all parts inside the loop. The maximum allowed drift of the specimen is 0.5 nm/min.



Main drift components and expansion loop.

For an impression of the required temperature stability, the thermal expansion loop is folded open; the total length is approximately 350 mm. If an average coefficient of thermal expansion is assumed for all the parts of 15 µm/m/K, the required temperature stability of the thermal expansion loop to meet the drift requirement of 0.5 nm/min is 0.1 mK/min. This temperature stability requirement is worst-case, since thermal expansions can cancel each other. However, the coefficients of thermal expansion and thermal time constants differ for all parts inside the expansion loop.

Main disturbances

The performance of electron microscopes is disturbed by mechanical vibrations and acoustics, and electromagnetic fields, but also due to thermal disturbances. These cause thermal-mechanical deformations of the system, which are observed in the image as drift. Thermal disturbances can be divided in external and internal disturbances. Main external disturbances are the air temperature variations in the electron microscope room and the temperature and flow variations of the cooling water. Main internal disturbances are temperature variations due to power dissipation variations of the electromagnetic lenses, motors and encoders.

A special case of disturbance is the insertion of a specimen holder. Typically, the temperature of the sample holder is not equal to that of the microscope. The sample holder has to take over the temperature of the microscope, and until a new thermal equilibrium is reached, the system will be subject to drift.

For counteracting acoustic disturbances high-end electron microscopes are placed in an acoustic enclosure, as shown in Figure 5. This acoustic enclosure also attenuates the effect of room temperature variations. The thermal time constant of such an enclosure is approximately 4 hours. This means that slow room air temperature variations, such as the day-night cycle, are still affecting the electron microscope, leading to thermally induced drift of the sample position with respect to the electron beam.

Thermo Fisher Titan microscope outside an opened acoustic enclosure. (Photo: Leo Koomen)

Power dissipation inside the sample manipulation stage due to motors and encoders, albeit only a few milliwatts, causes drift. The power dissipation of the electromagnetic lenses is also a main thermal disturbance. Although most electromagnetic lenses are operated in a constant-power setting, this is not applicable for all lenses inside the electron microscope. So, the variation in the power dissipation of the electromagnetic lenses is also a source of drift.

System identification

To meet the ever-increasing demands to enhance the throughput and positioning accuracy, thermal deformations must be analysed and compensated for using real-time error compensation techniques and an appropriate thermo-mechanical model. Accurate modelling of precise thermo-mechanical systems is complex, e.g., due to uncertain parameters and contact resistances. Earlier solutions to compensate for the deformations in electron microscopes, for instance, cannot cope with large deformations and strongly depend on model quality [5] [6]. Therefore, an accurate parametric model is desired for a model-based approach. Ideally, using a limited amount of temperature measurements combined with an accurate thermo-mechanical model enables the deployment of error-compensation techniques [7] [8].

State-of-the-art at Thermo Fisher

The state-of-the-art for thermal-mechanical system identification within Thermo Fisher is to apply step-like heat load excitations, and measure the response in temperature and/or drift. In certain scenarios, e.g., for measuring cooling-water-related transfer functions, a square-wave waveform is used as input signal, with a duty cycle of 50%, in which the time period of the waveform is varying.

Models are tuned (as yet) manually based upon the measured data in the time and frequency domain. The time constants of the system can be as long as 12 hours. Especially long time constants often result in experiments, either in the time or frequency domain, running for multiple days. During these measurements, the experiment is influenced by disturbances, including the varying ambient temperature. These influences often lead to poor signal-to-noise ratios, so that the information obtained from the experiment is limited.

Currently, experimental modelling of thermal systems is often done by sequential excitation of system inputs until steady state is achieved. Due to the large time constants in thermal systems, this method rapidly becomes tedious for an increasing number of inputs. There is a strong desire to reduce the time and to improve the quality of the measurements, and to improve the estimation of uncertain model parameters, such as the emissivity in radiation heat transfer, thermal contact resistances and material properties, e.g. at cryogenic temperatures.

Advances

Here, the key contribution lies in accurate modelling of thermomechanical behaviour using multi-input multi-output (MIMO) frequency response function (FRF) identification. Advances in system identification are leveraged to model thermomechanical systems and yield improved system models [9]. The approach is threefold and comprises the following contributions:

- Fast and accurate multivariable FRF estimations of thermal systems under transient conditions.
- Improved low-frequency estimation error by incorporation of additional sensor inputs.
- Estimation of thermal system parameters using a grey-box approach.

Transients

Consider a causal linear discrete time-invariant (LTI) system in an open-loop identification setting. The response $y(n)$ to an input $u(n)$ is given by:

$$y(n) = \sum_{m=-\infty}^{\infty} g(n-m)u(m)$$

Here, $g(n)$ is the impulse response of the system. Taking a measurement from t_{start} to t_{end} of length N and applying the discrete Fourier transform (DFT) yields:

$$Y(k) = G(\Omega_k)U(k) + T(\Omega_k)$$

Here, $\Omega_k = e^{\frac{-i2\pi k}{N}}$ with N the number of samples and $Y(k)$ and $U(k)$ the DFT of $y(m)$ and $u(m)$, respectively, and $G(\Omega_k)$ the frequency response function of the LTI system. Additionally, a term $T(\Omega_k)$ is required to account for the transient response by going from infinite time to a discrete time interval.

Traditionally, the empirical transfer function estimation (ETFE) is used to derive the FRF, defined as:

$$\begin{aligned}\hat{G}_{etfe}(\Omega_k) &= Y(k)U(k)^{-1} \\ &= G(\Omega_k) + T(\Omega_k)U(k)^{-1}\end{aligned}$$

Here, $T(\Omega_k)U(k)^{-1}$ is an estimation bias of the ETFE caused by transients in the response $y(n)$. While the ETFE can often yield acceptable results on mechanical systems, since the transient is significantly shorter than the measurement period, for thermal systems the estimation accuracy is severely biased due to the strong transients and large time constants, e.g. 4 hours for the acoustic enclosure. To reduce the estimation error, the transient should be explicitly addressed during the FRF estimation.

Local parametric modelling

To cope with data gathered under transient conditions, a local modelling method is adopted. The method is developed in [10] and applied in [11] and it uses a local rational parameterisation of $G(\Omega_k)$ and $T(\Omega_k)$. The system dynamics and transient are parametrised for a small local frequency window $k + r$ as:

$$G(\Omega_k) = \sum_{b=0}^{N_b} \theta_G B_b(k+r)$$
$$T(\Omega_k) = \sum_{b=0}^{N_b} \theta_T B_b(k+r)$$

Here, B_b are the basis functions and θ the corresponding estimation parameters. This parametrisation is linear in the parameters, i.e. the optimisation is convex with an analytic solution. Moreover, the basis functions B_b are user-specified, e.g. orthonormal rational functions. This combines the benefits of a linear optimisation and a rich, possibly rational, parameterisation. By explicitly estimating the transient term $T(\Omega_k)$ it can be removed from the FRF estimation of $G(\Omega_k)$, thus avoiding the estimation bias that would be obtained using the ETFE. Moreover, since transient data can be used, which is otherwise often discarded, a significant reduction in experimental measurement time is achieved.

Incorporating additional sensor inputs

One of the main environmental disturbances are the fluctuations in ambient temperature. To reduce the effect of these disturbances on the system identification set-up, measurements of the ambient temperature are incorporated as an additional input. In particular:

$$Y(\Omega_k) = \hat{G}(\Omega_k)\begin{bmatrix}U(k)\\D(k)\end{bmatrix} + T(\Omega_k)$$

Here, $D(k)$ is the DFT of the measured environmental disturbance, e.g. the ambient temperature. Here, $\hat{G}(\Omega_k)$ is now a 1x2 multi-variable transfer function matrix since it includes an additional transfer function, i.e. $\hat{G}(\Omega_k) = [G(\Omega_k)_{u_1 \to T_1} \quad G(\Omega_k)_{T_\infty \to T_1}]$. By using the proposed local parametric method, this full transfer function matrix is estimated from the measurement data. Since the ambient temperature typically contains the most energy at lower frequencies, including this as an additional 'excitation' input removes a low-frequency disturbance and consequently leads to improved estimation results for this frequency range.

Parameter estimation

A lumped-parameter model is often used for initial analysis during the design process, and initial prototyping stage. To facilitate model-based control and error compensation approaches, an accurate parametric model of the thermo-mechanical system is desired. The lumped-parameter model often contains parameters and boundary conditions that are uncertain or unknown, e.g. material properties or thermal contact resistances. At present, models are tuned manually based upon the measured data in the time and frequency domain. With increasing complexity of the physical systems, and their corresponding models, the manual tuning of parameters is becoming too cumbersome.

Grey-box identification

To yield high-fidelity thermomechanical models, grey-box identification is used to improve the accuracy of unknown parameters in the lumped-parameter models. By means of spatial discretisation of the thermal dynamics a parameterised model is generated, here shown in state-space form:

$$G(\Omega_k, \phi) := \begin{cases} T(t) = & A(\phi)T(t) + B(\phi)u(t) \\ y(t) = & C(\phi)T(t) \end{cases}$$

Here, $\phi \in R^{N_p x 1}$ is the parameter set with N_p the number of parameters. The aim of grey-box identification is to calibrate the parameter set ϕ such that the model is suitable for control. The approach is based on minimising the discrepancy between the measured non-parametric FRF and the FRF of the parametric model with the following cost function:

$$J(\phi) = \min_{\phi} \left\{ \left\| W(\Omega_k) \left(\hat{G}(\Omega_k) - G(\Omega_k, \phi) \right) \right\|_2^2 \right\}$$

Here, $\hat{G}(\Omega_k)$ is the measured FRF, $G(\Omega_k, \phi) = C(\phi)\left(\Omega_k - A(\phi)\right)^{-1} B(\phi)$ is the FRF of the parametric model and $W(\Omega_k)$ is a dynamic weighting filter based on the variance of the measured FRF. By minimising the cost function J the parameter values in ϕ become such that the parametric model best describes the experimental system. This yields a high-fidelity model suitable for advanced control and error compensation techniques.

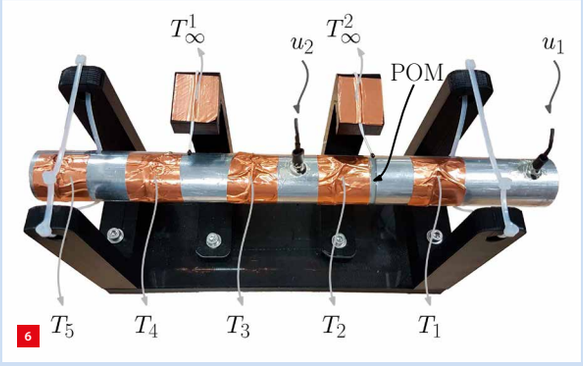
Case study

The presented approaches for system identification are applied to a 1D thermal system; see the box on the right.

(Main article continued on page 18.)

Case study: 1D thermal system

The experimental set-up shown in Figure 6 consists of an aluminium cylinder containing a slice of high-thermal-resistance material (POM), two excitation inputs (u_1, u_2), two temperature sensors (T_i, $i \in [1,5]$) and two ambient temperature sensors (T_∞). The experimental set-up is representative of a chain of thermal resistances in 1D, a situation commonly found in electron microscopes where the thermal expansion is considered dominant in one direction; see, e.g., Figure 4.



6

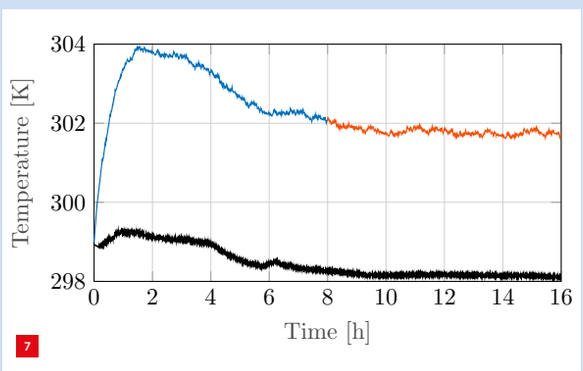
Experimental set-up. An aluminium cylinder containing a slice of high-thermal-resistance material (POM), two excitation inputs (u_1, u_2), two temperature sensors (T_i, $i \in [1,5]$) and two ambient temperature sensors (T_∞).

Identification under transient conditions

The local parametric method has the potential to construct a system FRF from data obtained under transient conditions. For this, the heater u_1 and sensor T_1, shown in Figure 6, are used as input and output, respectively. The excitation signal $u_1(t)$ is a random-phase multi-sine, i.e. a collection of sinusoidal signals:

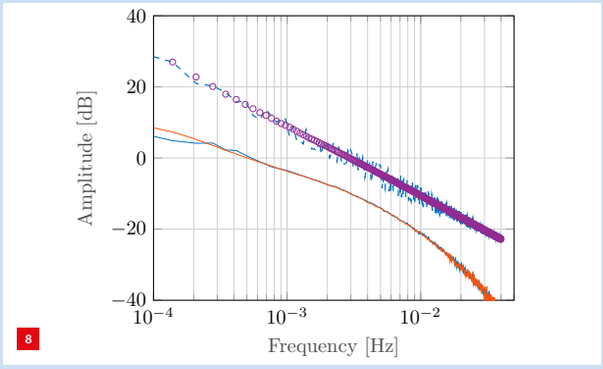
$$u_1(t) = \sum_{k=1}^{N} A_k \sin\left(\frac{2\pi k t}{N} + \psi_k\right) + \Delta$$

Here, N is the amount of samples in one period, A_k is an amplitude, ψ_k a uniformly distributed phase on $[0,2\pi)$ and Δ an off-set since the input is constrained to be positive. By then applying 4 periods of each 4 hours as excitation, a time-domain response as shown in Figure 7 is obtained.

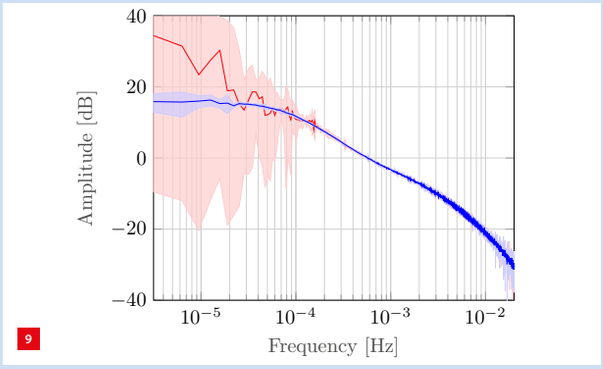


7

Temperature response $u_1 \rightarrow T_1$ of the experimental set-up to a random-phase multi-sine with offset for 4 periods of each 4 hours. The dataset is divided into two sub-records, (1) containing the first two periods (in blue), and (2) containing the last two periods (in red), considered as a validation data-set. A measurement of the ambient temperature T_∞ is shown in black.



FRF estimation using the ETFE (blue dashed) and the proposed method (blue solid). It shows that the ETFE clearly estimates an erroneous FRF when compared to the validation data (red solid), while the proposed method does not. This is caused by the transient component $T(\Omega_k)$, indicated as magenta circles.



FRF estimation of $u_j \rightarrow T_i$ by (a) using only input u_j (red); and (b) incorporating additional inputs (blue), thereby reducing the impact of environmental disturbances on the FRF estimation. This results in an improved low-frequency FRF estimation, since these disturbances typically contain most of their energy in this region.

The time-domain response shows an initial step-like response in temperature, due to the offset Δ in u_1, in addition to a periodic response to the multi-sine excitation. Two sub-records of the same dataset are considered:

- The first sub-record includes the first two periods, containing a significant initial transient and environmental disturbances.
- The second sub-record consist of the last two periods with a substantially smaller transient and environmental disturbance, and is used as a validation dataset.

Applying both the proposed local parametric identification method and the ETFE on the first sub-record of the data in Figure 7 yields results as shown in Figure 8. Both methods are compared to the FRF obtained by applying the proposed method on the second sub-record, which is considered a validation dataset. It then shows that the ETFE is severely biased by the transient component $T(\Omega_k)$, shown as magenta circles, while the proposed method is not.

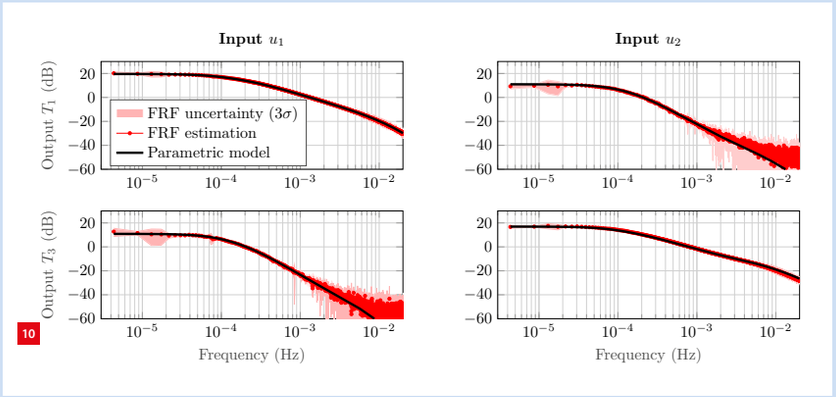
This illustrates that the proposed method is insensitive to the initial transient in the data set and estimates an FRF that is almost identical to the one obtained from the validation record. This potentially leads to significant savings in experimental time, since now data obtained under transient conditions can be used that would otherwise be discarded.

Incorporating additional inputs

Incorporating additional input signals can potentially yield an improved FRF estimation by increasing the energy in the system. The results in Figure 9 illustrate effects of including the ambient temperature T_∞ as an additional input. It shows that the low-frequency estimation is improved and a smaller variance is achieved, as indicated by the shaded area.

Grey-box parameter estimation

The cumulative effort of the previous techniques yields an accurate FRF suitable for parameter calibration. The parameters of a multi-input multi-output (MIMO) lumped-capacity thermal model are calibrated by minimising the cost function $J(\varnothing)$ using a Nonlinear Least Squares optimisation procedure in MATLAB. In Figure 10 the estimated non-parametric FRF and the calibrated parametric model are shown. Clearly, the estimated parametric model is within the 3σ uncertainty of the FRF estimation.



Non-parametric FRF estimate (dotted) of the experimental set-up and the 3σ estimation uncertainty (red shaded). The FRF is used for a grey-box parameter estimation, yielding a high-fidelity parametric model (black solid)

Moreover, it shows that the transfer functions on the off-diagonal have a reduced gain level and an increased estimation uncertainty. This is the result of the slice of POM material glued in between the two aluminium parts of the beam, as shown in Figure 6. The POM material has a lower conductivity, therefore acting as a high thermal resistance between $u_1 \rightarrow T_3$ and $u_2 \rightarrow T_1$ making the identification of the related transfer functions increasingly difficult due to the reduced signal-to-noise ratio. The proposed calibration procedure yields a MIMO high-fidelity parametric model of the experimental system that is suitable for advanced control techniques and error compensation strategies that enable increased attenuation of thermal-induced deformation errors.

Summary

Drift caused by thermal expansion in an electron microscope is one of the leading sources of error in the final imaging performance. Moreover, due to the ever-increasing demands to enhance the throughput and positioning accuracy, the specifications for the drift requirements are increasingly stringent. This necessitates a thorough analysis of the thermal effects and an appropriate control approach using an accurate thermomechanical model. Accurate modelling of precise thermomechanical systems is complex, e.g., due to uncertain parameters and contact resistances.

The identification framework presented in this article enables the fast and accurate identification of thermal dynamics in view of precision motion control. The proposed methodology has been applied to a multi-variable experimental set-up. It achieved a significant improvement in estimation accuracy and a reduced experimentation time by suppressing the transient and disturbance contributions. The presented methods facilitate the implementation of advanced control techniques and error compensation strategies, enabling increased accuracy and throughput in electron microscopy and other high-precision mechatronic systems.

REFERENCES

[1] TEM intro for Non-Technical employees ILT, Thermo Fisher internal course.

[2] "An introduction to electron microscopy", *www.fei.com/WorkArea/DownloadAsset.aspx?id=15032385923*

[3] D.T. Spaan-Burke, "Advanced Thermal Control Consortium", *www.ibspe.com/public/uploads/content/files/ATCTier%203%20Flier%20Aug%202016.pdf*

[4] E. van Horssen, "Data-intensive feedback control: switched systems analysis and design", Ph.D. thesis, Eindhoven University of Technology, 2018.

[5] B.S. Salmons, D.R. Katz and M. L. Trawick, "Correction of distortion due to thermal drift in scanning probe microscopy", *Ultramicroscopy*, vol. 110, no. 4, pp. 339-349, 2010.

[6] A.N. Tarau, P. Nuij and M. Steinbuch, "Hierarchical control for drift correction in transmission electron microscopes", in *2011 IEEE International Conference on Control Applications (CCA)*, Denver, CO, USA, 2011.

[7] E. Evers, M. van de Wal and T. Oomen, "Synchronizing decentralized control loops for overall performance enhancement: A youla framework applied to a wafer scanner", in *20th IFAC World Congress*, Toulouse, France, 2017.

[8] A.H. Koevoets, H.J. Eggink, J. van der Sanden, J. Dekkers and T.A.M. Ruijl, "Optimal sensor configuring techniques for the compensation of thermo-elastic deformations in high-precision systems", in *13th International Workshop on Thermal Investigation of ICs and Systems (THERMINIC)*, 2007.

[9] E. Evers, N. van Tuijl, R. Lamers and T. Oomen, "Identifying Thermal Dynamics for Precision Motion Control", submitted for conference publication, 2019.

[10] E. Evers, B. de Jager and T. Oomen, "Improved local rational method by incorporating system knowledge: with application to mechanical and thermal dynamical systems", in *18th IFAC symposium on system identification*, Stockholm, 2018.

[11] E. Evers, B. de Jager and T. Oomen, "Thermo-Mechanical Behavior in Precision Motion Control: Unified Framework for Fast and Accurate FRF Identification", in *IECON 2018 - 44th Annual Conference of the IEEE Industrial Electronics Society*, Washington, DC, USA, 2018.