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Pressure-induced cavity deformation in Fabry-Pérot refractometry - Characterizations and Recommendations

Report on the activity A1.1.4 in the EMPIR project 18SIB04, "QuantumPascal".

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Abstract Fabry-Perot (FP) cavity based refractometers are subjected to pressure-induced deformation when exposed to gas that changes their lengths. Unless this is taken into consideration properly, pressure assessments can be adversely affected. It is therefore of importance to accurately assess the amount of deformation of such cavities. Two major means of doing this are simulations and experimental characterizations. In the EMPIR project "QuantumPascal", several FPC systems have been characterized with respect to their pressure-induced deformation, $(\Delta L/L)/P$, by simulations. It was found that their pressure-normalized relative deformation ranges over more than a factor of 35, from 0.2×10^{-12} to 7.8×10^{-12} Pa^{-1}. More importantly, several of these characterizations were found to provide assessments of the deformation that are limited by either the ability to model the system in the simulation program or the uncertainty in the material parameters used, e.g. Young's modulus and Poisson ratio, which often are in the percentage to permille range. Only two simulations demonstrated assessments of deformation with an uncertainty that allows for assessments of pressures with the 10 ppm targeted relative uncertainty. Experimental characterizations do not suffer from the same type of limitations. On the other hand, they are often restricted by various types of external disturbances. As a means to mitigate such, a novel robust methodology has been developed that allows for assessments of cavity deformation that are independent of systematic pressure-independent errors in both the reference pressure and the assessment of gas temperature, and, when carried out by use of the gas modulation refractivity (GAMOR) methodology, also is insensitive to gas leakages and outgassing. It was demonstrated that when a high-precision (sub-ppm) refractometer is characterized according to this methodology, and when high purity gases are used, the uncertainty in the deformation solely contributed to the uncertainty in the assessment of pressure of N_2 with 1 ppm, thus allowing it to be assessed in an otherwise well-characterized system well within the 10 ppm targeted uncertainty. This methodology was, in this project, applied to the assessment of deformation in several FPC systems. In total, four FPC systems were characterized by various experimental means. Recommendations for how to realize FP-based refractometer systems with a minimum of deformation are given.

Contents

1 Introduction

Realized in a proper manner, refractometry can be used to assess not only refractivity but also, by the use of the Lorentz-Lorenz equation and an equation of state, molar density and pressure. The most sensitive refractometers are based on Fabry-Perot (FP) cavities in which a laser is used to probe the frequency of a longitudinal mode [1–7]. Since frequency is the entity that can be assessed with highest accuracy in our society [8–10], FPC-based refractometry has a great potential for accurate assessment of pressure [11–20].

Although many realizations of such refractometers have shown promising results, a crucial limiting issue that needs to be addressed is the fact that the cavities are subjected to pressure-induced deformation when they are exposed to gas pressure that will change their lengths. Without taking this effect into consideration properly, pressure assessments can be adversely affected, up to the permille range. It is therefore of importance to accurately assess the amount of deformation in FP-cavities used for refractometry.

One way to do this is to use simulations, preferably using finite element methods (FEMs). By simulating a cavity spacer system with a given set of geometric and material parameters, and comparing the cases with and without gas in the cavity, the pressure-induced deformation can be estimated. However, simulations are often limited by the finite accuracy by which the system can be modelled and various material properties are known.

Another means comprise experimental characterizations of the systems. Since the refractive index of helium can be calculated accurately from first principles, and its value differs from that of most other gases by almost one order of magnitude, often advocated methods for assessment of cavity deformation are based on the use of this gas.

In the simplest form, originally proposed by Stone and Stejskal [11], helium gas is addressed at a known pressure and the deformation is assessed in terms of the difference between the measured and the theoretically predicted refractivity.

Another method used for experimental characterizations of pressure-induced deformations is to utilize a detection methodology in which the influence of deformation is automatically canceled. Such a technique, also originally proposed by Stone and Stejskal [11], is to utilize two gases; rather than tracking the change in refractive index as the cavity is evacuated (i.e. to a situation for which $n = 1$), one should instead assess the change in refractivity when the gas addressed is replaced by helium at the same pressure.

A variation of this technique, denoted the "two-gas method", was proposed by Egan et al. [21]. In this methodology, the deformation is assessed by performing measurements of the refractivity of two gases with different (but known) refractivity at the same pressure assessed by the use of an evaluation model that does not take deformation into account [21]. Since the two measurements are affected by a common error, given by the deformation, and the ratio of the refractivity of the two gases are known, the deformation can be unequivocally deduced.

Although all these experimental approaches look straightforward, it is far from trivial to utilize any of them if deformation is to be assessed by the accuracy that is needed to obtain low uncertainty assessments of pressure. They require either, when a single gas (He) is used, that the empty cavity optical length has been accurately assessed, or, when a two-gas method is used, that the refractivities of both gases are known at at least one pressure. In all cases, they are often limited by various types of drifts, gas impurities, and outgassing.

There are two ways around this. One is to create FP cavities with a minimum of (or even no) deformation. The justification for this is that, the smaller the deformation is, the less relative accuracy it needs to be determined with if cavity deformation should not contribute more than a given amount to the uncertainty of an assessment of refractivity (or pressure). A disadvantage of this is that the cavities design might become complex.

Another is to develop and utilize a measurement methodology that properly can assess the deformation with such high accuracy that its uncertainty has a minimal influence of the assessment of refractivity or pressure. An advantage of this is that a larger variety of cavities can be assessed with respect to their deformation.

The EMPIR 18SIB04 ”QuantumPascal” project, titled "*Towards quantum-based realisations of the pascal*", was initiated 2019 with the overall aim to "*develop novel quantum-based pressure standards based on optical, microwave and dielectric methods and to assess their potential with the aim of replacing the ex-*

isting mechanical based pressure standards". Its first work package, WP1, was devoted to "*Pressure measurements based on Fabry-Pérot cavity based refractometry*".

Task 1.1 in this work package was devoted to "*Fabry-Perot cavity deformation*". Its main aim has been to characterize cavities with respect to deformation (by simulations or experimental means) sufficiently well so they do not significantly affect the uncertainties of pressure assessments (more precisely, so that pressure can be assessed with a targeted uncertainty of 10 ppm) and, if possible, to propose cavity designs that exhibit a minimum amount of deformation.

To be able to accurately characterize cavities with respect to deformation by experimental means, a novel disturbance-resistant characterization methodology has been developed that has proven to be able to assess deformation in high-precision refractometry systems with such high accuracy that it solely marginally contributes to the uncertainty of pressure when nitrogen is addressed [22]. This has decreased the immediate need for design and construction of FP-cavities with a minimum of deformation, wherefore the work in this work package has been focused upon the characterization of existing FP-cavities with respect to their pressure-induced deformation based on FEM-based calculations and experimental characterizations.

2 Theory

2.1 Influence of cavity deformation on the assessment of refractivity

As is shown by Eq. (13) in Silander et al. [23], it is possible to express, in the presence of the Gouy phase and the mirror penetration depth, with a minimum of approximations (which are on the 10^{-9} to low 10^{-8} level), the refractivity, $n-1$, in terms of measurable quantities and material parameters as

$$n-1=\frac{\frac{\Delta\nu}{\nu_0}(1+\frac{\Theta_G}{\pi m_0}+\frac{\gamma_c}{m_0})+\frac{\Delta m}{m_0}}{1-\frac{\Delta\nu}{\nu_0}(1+\frac{\Theta_G}{\pi m_0}+\frac{\gamma_c}{m_0})+\frac{\Theta_G}{\pi m_0}+n\varepsilon'} \approx \frac{\frac{\Delta\nu}{\nu_0}(1+\frac{\Theta_G}{\pi m_0}+\frac{\gamma_c}{m_0})+\frac{\Delta m}{m_0}}{1-\frac{\Delta\nu}{\nu_0}(1+\frac{\Theta_G}{\pi m_0}+\frac{\gamma_c}{m_0})+\frac{\Theta_G}{\pi m_0}}(1-n\varepsilon'), \quad (1)$$

where we, in the first step, have introduced ε' as the refractivity-normalized relative elongation of the cavity due to the presence of the gas, defined as $(\Delta L/L)/(n-1)$, where, in turn, ΔL is the change in length of the cavity due to the gas pressure and L is the length of the cavity (in vacuum) experienced by the light during scans, and where the other entities have their standard interpretation.[1] The second step originates from a series expansion of the first expression in term of $n\varepsilon'$ (which is valid for all normal types of cavities).

As also is shown in Silander et al. [23], making use of the definition of ε', it is possible to alternatively write the latter expression as

$$n-1=\frac{\frac{\Delta\nu}{\nu_0}(1+\frac{\Theta_G}{\pi m_0}+\frac{\gamma_c}{m_0})+\frac{\Delta m}{m_0}}{1-\frac{\Delta\nu}{\nu_0}(1+\frac{\Theta_G}{\pi m_0}+\frac{\gamma_c}{m_0})+\frac{\Theta_G}{\pi m_0}}-n\frac{\Delta L}{L}. \quad (2)$$

This shows that there are naturally two similar (and to a certain degree equivalent) entities that mediate the amount of deformation in FP-based refractometry; a refractivity-normalized relative elongation, ε', and a relative elongation, $\Delta L/L$, evaluated at the pertinent pressure.

Equation (1) shows that while the refractivity-normalized relative elongation, ε', is a measure of the *relative* change of the assessed refractivity due to deformation, the relative elongation, $\Delta L/L$, represents the corresponding *absolute* change in refractivity. Although the latter one is naturally the most commonly used entity when simulations are performed [most often expressed in terms of κP, where κ is a pressure-normalized relative elongation, $(\Delta L/L)/P$, assessed by simulations], the former is particularly useful in the novel experimental deformation-characterization methodology recently developed [22] since it has several advantages. One is that its value is virtually pressure independent, which facilitates the assessment of refractivity for various pressures.[2] Another is that it directly, by its value, assesses the relative influence of deformation

[1] $\Delta\nu$ is the shift in the frequency of the laser that takes place when the gas is let into the cavity, ν_0 is the frequency of the mode of the cavity the laser addresses in the absence of gas, Θ_G is the single pass Gouy phase, m_0 is the mode number addressed in an empty cavity, γ_c is a fully material-dependent entity related to the penetration depth of the mirrors, that, for an ideal quarter wave stack (QWS), is given by $(n_H-n_L)^{-1}$, Δm is the number of modes the laser has jumped during the filling (or emptying) of the cavity, L is given by $L_0+2L_{\tau,s}$ where L_0 is the distance between the front facets of the DBRs coatings of the two mirrors and $L_{\tau,s}$ is the frequency penetration depth of a QWS that, in turn, is related to γ_c through $\frac{c\gamma_c}{4\nu_c}$.

[2] While Eq. (1) can directly be used when a variety of pressures

on the assessments of refractivity and pressure; e.g. a system with an ε' of 10^{-4} is influenced by deformation on the 100 ppm level. This also implies that its uncertainty, i.e. $\delta\varepsilon'$, represents the relative uncertainty in the assessment of refractivity and pressure, i.e. $\delta(n-1)/(n-1)$ and $\delta P/P$, respectively.

2.2 Benchmarks for the cavity deformations

A necessary prerequisite for an assessment of pressure with a (relative) uncertainty of 10 ppm is that also the refractivity needs to be assessed with (at least) the same (relative) uncertainty.[3] To achieve this, Eq. (1) then indicates that the refractivity-normalized relative elongation of the cavity, i.e. ε', needs to be assessed with (at least) the same (absolute) uncertainty, in this case with 1×10^{-5}.

Since, to first order, pressure, P, is related to refractivity by $P = RT\frac{2}{3A_R}(n-1) = \zeta(n-1)$ where R, T, and A_R are the gas constant, the temperature, and the molar polarizability of the gas addressed, respectively, the pressure-normalized relative deformation of the cavity, κ, is related to ε' as ε'/ζ. Moreover, since, for nitrogen, ζ takes a value of $3.73371(3) \times 10^8$ Pa [22],[4] this implies that, to allow for an assessment of pressure with an uncertainty of 10 ppm, a necessary requirement is that the pressure-normalized relative deformation of the cavity, i.e. κ, needs to be assessed with a maximum (absolute) uncertainty of 2.7×10^{-14} Pa^{-1}.[5]

These two requirements, i.e. an ε' of 1×10^{-5} and a κ of 2.7×10^{-14} Pa^{-1}, will henceforth be referred to as the "benchmarks" and be the values to which all simulated or experimental deformation assessments in this guide are to compared.

3 Characterization by simulations

3.1 Initial scrutiny

The initial activity within task 1.1, referred to as A.1.1.1, dealt with simulations of the pressure-induced deformation of a given Fabry-Pérot cavity using various versions of two types of software, COMSOL Multiphysics® and ANSYS Workbench [24]. The main aim of this activity was to certify that all partners were using adequate modeling tools in a proper manner.

It was demonstrated, by four participants of the project, that simulations of the deformation could be performed adequately by the use of dissimilar software and versions of those, with such small discrepancies that the 95% confidence interval of the simulated pressure-induced axial deformation only would contribute to a sub-ppm discrepancy in refractivity assessments of N_2 [24]. This excellent, software-independent agreement of the simulation results ensures that a design with a lower simulated pressure-induced deformation in reality should have a lower pressure-induced deformation, allowing for direct and software-independent comparisons of simulation results and designs.

3.2 Basic dependencies

To gain a basic understanding of the concept of cavity deformation, simulations of a single closed cavity[6] were performed with particular regard to the dependence on three parameters, viz.

1. The radius r of the bore of the cavity;
2. The thickness d of the mirror substrate (which is also the sealing plate of the cavity); and
3. The length L of the cavity.

As is illustrated in Fig. 1, for symmetry reasons, only one eighth of the cavity was considered (one half per dimension). The spacer and the mirror substrates were assumed to be made of the same isotropic material. Since this simulation was made to

are to be assessed, Eq. (2) requires knowledge about the pressure to be assessed on beforehand (so as to assess the value of $\Delta L/L$). This prevents its use for automated assessment of sets of unknown pressures.

[3]Note that this is not a sufficient conditions, since also entities such as the molar polarizability, the virial coefficients, and the assessment of temperature can have associated uncertainties. However, since the latter entities were not addressed in Task 1.1 of the "QuantumPascal" project, the study presented here was solely focused on the requirements to reach the necessary prerequisite to assess the refractivity with the same (relative) uncertainty as that of the pressure.

[4]This value is strictly valid only for a wavelength of 1.55 µm and at 30 °C. Although ζ has a dependence on both the wavelength and the temperature, it is, over the relevant ranges of these entities, very weak.

[5]For comparison, for 100 kPa, and, for the system considered in section 3.2 below, i.e. for a 0.05 m long cavity, the latter corresponds to an uncertainty in length of 1.4×10^{-10} m (i.e. 0.14 nm).

[6]The concept of "closed cavity" refers to a system that solely fills the cavity with gas, not the space outside the spacer.

gain a general understanding of the concept of cavity deformation, the exact material properties were considered to be secondary and, for simplicity, the material parameters for Invar (used in some simulations, see below) were used. Mirrors and cavity spacer were assumed to be in direct contact, as would be the case be for optical contacting.

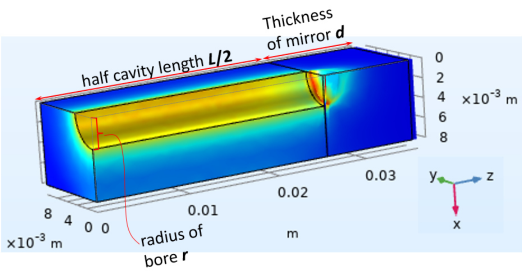

Figure 1. Simple model of a spacer and a mirror presented by rectangular cuboids. The point [0,0,0] represents the center of symmetry. Therefore, only 1/8 of the geometry (and only a part of one mirror) needed to be simulated.

Here, the simulated pressure-dependent length of the measurement FP-cavity, $L(P)$, is given by two times the distance between the center of symmetry, [0,0,0], and the surface of the mirror in the center, which is at [0, 0, $L/2$], without any pressure inside the cavity. To simulate the length change of a dual FP-cavity (DFPC), i.e. a spacer also comprising a reference cavity, also the distance of the spacer between the points at [8 mm, 0, 0] and [8 mm, 0, $L/2$] was considered to represent the deformation of the reference cavity.[7]

Although the actual dependencies of the cavity deformation on the aforementioned parameters are rather intricate, it is possible to assess the main dependence on each parameter separately as done in the following subsections. The basic parameters of the modelling are given in Table 1.

3.2.1 Dependence on the radius r of the measurement cavity

For a closed cavity, it is expected that the pressure-induced elongation of the measurement cavity should predominantly be proportional to the cross-sectional area of the bore, thus that it is has a quadratic dependence on the radius. However, due to effects such as the amount of spacer material over which the force is distributed and mirror bending, the actual dependence will differ slightly from this. This is illustrated by the blue markers in Fig. 2, which illustrate the pressure elongation of the measurement cavity as a function of the radius of the cavity bore. Although the response is mainly quadratic, it requires a higher order polynomial (in this case a fourth order) to accurately describe the response.

[7] Note that, for simplicity, without actually modelling any reference cavity, the simulations treated the distance between the points in the spacer at [8 mm, 0, 0] and [8 mm, 0, $L/2$] as a measure of the deformation of the reference cavity.

Table 1. Parameters of the simulated FP-cavity in Fig. 1 used to gain an basic understanding of the concept of pressure-induced distortion.

Parameters	Value
Half spacer width in the "x"-direction	8 mm
Half spacer height in the "y"-direction	10 mm
Half spacer length "$L/2$" in "z"	25.5 mm
Distance between the two cavities	8 mm
Thickness of mirror "d"	30 mm
Radius of bore "r"	3 mm
Initial pressure "p_0"	0 kPa
Final pressure "p_{max}"	100 kPa

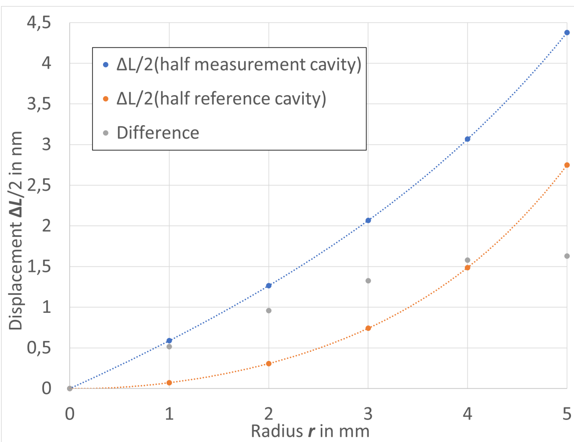

Figure 2. Pressure-induced elongation of the measurement and reference cavities as a function of the bore radius of the measurement cavity, r.

The data displayed in red show the corresponding associated distortion of the empty reference cavity when the measurement cavity is filled with gas. The data show that also the reference cavity in a DFPC system will change its length when the measurement cavity gas is filled with gas.[8] It can be concluded though that this elongation has a weaker dependence on the radius of the measurement cavity; it is virtually negligible for the smallest bore radii and take noticeable values only for larger ones. It can also be noticed that the difference in elongation of the two cavities (shown by the grey markers in Fig. 2) will, for increasing radii, approach a limit value corresponding to the bending of the mirror surfaces in the measurement cavity.

This implies that one means to minimize the pressure-induced deformation is to use an as small bore radius as possible. It should be noticed though that this does not apply to open cavities, in which the spacer is affected by pressure from both the inside and outside, since, in that case, the net area over which gas is acting on the spacer is larger. This also implies that the pressure-induced deformation is, in general, larger for open than for closed systems.

3.2.2 Dependence on the thickness d of the mirror

The dependence of the pressure-induced elongations of the measurement and reference cavities on the thickness of the mirrors substrates (which are also the sealing plates of the measurement cavity), i.e. d, are shown in Fig. 3. The data indicate that the elongation has two origins; one from the elongation of the spacer (which dominates for large mirror thickness) and another from the compression and bending of the mirror substrates (providing the main dependence for small d).

The deformation of thin mirrors is considerable, which indicates that such mirrors have a substantial effect on the pressure-induced elongation of the cavity. In this particular case, the mirror bending leads, for a 1 mm thick substrate, to an elongation of more than 16 nm while it, for substrates that are thicker than 4 mm, only contribute with an elongation that is 2 nm. It can be concluded from the data that for substrates thicker than the diameter of the cavity

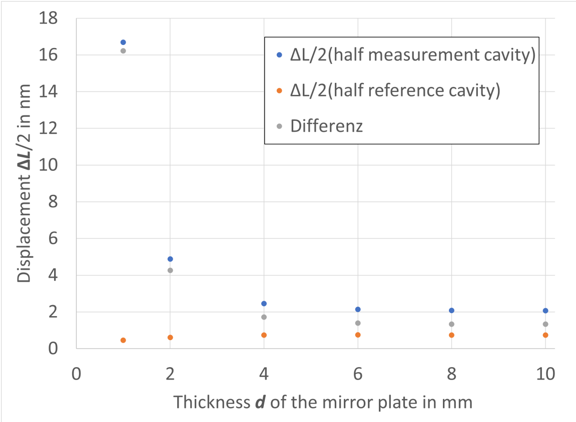

Figure 3. Pressure-induced elongations of the measurement and reference cavities for mirror plates with different thickness d when gas is filled into the measurement cavity.

bore, which in this case is 6 mm, there is virtually no dependence on the mirror thickness. For example, for the case when the thicknesses are 10 and 50 mm, the deformations are 2.072 and 2.086 nm, respectively. This shows that the deformation of the mirrors will not be markedly reduced by thickening the substrates beyond the diameter of the cavity.

3.2.3 Dependence on the length L of the cavity

The dependence of the pressure-induced elongations of the measurement and reference cavities on the cavity length, i.e. L, are shown in Fig. 4.

The data show that also in this case does the elongation consists of two parts; one that is proportional to the length of the spacer (or at least a part of it) and one that depends mainly on the deformation of the mirrors.

As is shown in Fig. 5, since the mirrors are bonded to the spacer, the mirror deformation will affect also the parts of the spacer close to the mirrors (represented by the parts of the spacer that are outside the red rectangle). This implies that, by comparing multiple systems with dissimilar lengths, or changing the length of a system with adjustable length, it should, in principle, be possible to separately assess pressure-induced deformations of the cavity spacer and the mirrors. Attempts in this direction have been suggested and performed by Ricker et

[8] Exposing one cavity in a DFPC system to gas pressure will affect the length of both cavities, although to dissimilar extent. Since it is the net change in length between the two cavities that will affect the measurements, the deformations simulated are likewise given as the "net" deformation, i.e., as the difference in the change in length between the two cavities.

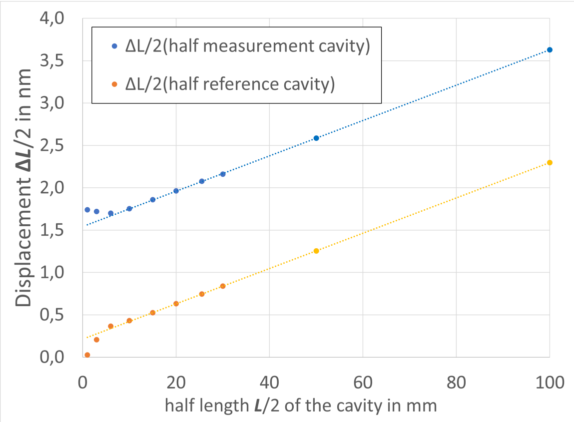

Figure 4. Pressure-induced elongation of measurement and reference cavities for spacers with different lengths L when gas is filled into the measurement cavity.

al. [25] and Takei et al. [26]. However, since such assessments often are limited by the mechanical stability or manufacturing tolerances, their accuracy has have so far not been impressive. This implies that this methodology should be exercised with caution.

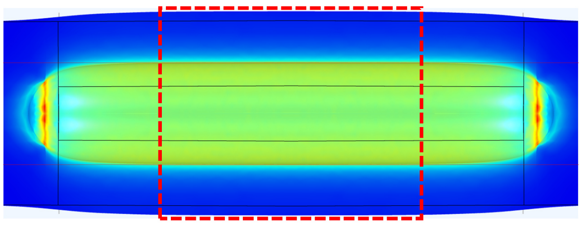

Figure 5. Illustration of the pressure-induced elongation of the measurement cavity. The part inside the red rectangular is responsible for the linearly contribution to the elongation in Fig. 4.

3.3 Net zero deformation dual FP cavity (DFPC) systems

UmU and PTB investigated, by use of simulations, possible means to create single FP-cavity systems with no (or a minimum of) net cavity deformation [based on a balancing of the pressures (in reality the forces) created by the gas inside and outside the cavity]. To obtain a zero net cavity deformation i DFPC systems, the simulations strove for equal pressure-induced length changes of the measuring and reference cavities. Possible means to realize such systems were identified and investigated.

The simulations indicated though that the designs become rather complex. One such example, realized in a sapphire-based system, is shown in Fig. 6.

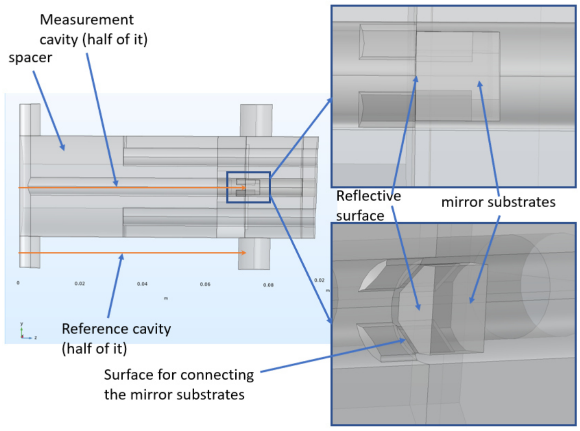

Figure 6. An example of a possible net zero deformation DFPC system.

It was concluded that such designs cannot be implemented at a reasonable cost due to complex structures and stringent manufacturing tolerances. Since the results of the experimental characterizations using the two-gas method (see below) were successful, the work on the zero deformation cavities was discontinued.

3.4 Simulations of existing cavities

Four partners of the "QuantumPascal" project, UmU, PTB, CNAM, and CEM, were then simulating different types of cavities with varying geometries made from the presently most commonly used (as well as novel) spacer materials (Zerodur, Invar, and sapphire), representing cavity systems in which experimental characterizations were subsequently planned to be performed. All simulations addressed the deformation caused by nitrogen gas.

3.4.1 Simulations of closed dual FP cavity (DFPC) systems at UmU and RISE

Two different existing cavity spacer systems comprising dual Fabry-Perot cavities (DFPC) were simulated with respect to the influence of some macroscopic entities of the cavity spacer block and the mirrors[9] on their longitudinal pressure-induced deformation. One of the spacers, used in early works with the Gas Modulation Refractometry (GAMOR) methodology, was made of Zerodur [18, 19], while the other, which has been used in the more recent activities, was made of Invar [27–32, 23].

The simulations were performed with COMSOL Multiphysics®, version 5.5, together with the structural mechanics module, the nonlinear structural materials module, the CAD import module, and the LiveLink for Inventor module.

3.4.1.1 A closed DFPC system realized in a Zerodur spacer at UmU

The two cavities in the Zerodur spacer consisted of 6.1 mm wide 190 mm long bores, separated by 50 mm. In the simulations, the mirrors were, for simplicity, assumed to be flat and mounted by optical contacting on each side of the bores. The longitudinal displacements of the center points of the mirror surfaces were assessed for each cavity separately, as well as for their difference, when the measurement cavity was exposed to a pressure of 100 kPa [33].

The simulations provided a net pressure-normalized relative deformation, κ, of 0.76(2) $\times 10^{-12}$ Pa^{-1}, corresponding to a pressure-normalized relative deformation, ε', of 2.8(1) $\times 10^{-4}$, where the uncertainty comes from the uncertainty in the material parameters, i.e. Young's modulus and Poisson ratio [33]. This implies that the uncertainties in the relative deformations, which for the pressure-normalized relative deformation was estimated to 2×10^{-14} Pa^{-1}, are just within the required benchmark (which is 2.7×10^{-14} Pa^{-1}).

The simulations also comprised a parametric study of the role of three geometrical properties on the deformation, viz. the cavity diameter, the mirror thickness, and the cavity separation. It was found, in agreement with the study presented in section 3.2 above, that the cavity diameter plays the largest role of these — as expected, increasing the cavity diameter by a factor of $\sqrt{2}$, so as to double the area of the mirror the gas is acting on, almost doubled the deformation, to a value of $1.22(3) \times 10^{-12}$ Pa^{-1}, additionally aggravating the ability to assess pressure with an overall uncertainty of 10 ppm — and that the deformation was significantly affected by the thickness of the mirrors only when they were thin (in this particular case, thinner than half of its real thickness). It was additionally found that the cavity separation plays a minor role on the net deformation [33].

3.4.1.2 Closed DFPC systems realized in Invar spacers at UmU and RISE

The second study was performed on a closed DFPC system made of Invar,[10] used by both UmU and RISE, shown in Fig. 7, comprising two 148 mm long and 6 mm wide cavities, separated by 25 mm. The spacer was made from an Invar rod with a diameter of 60 mm. Each cavity consists of two ∅12.7 mm highly reflective (99.997%) plano-concave mirrors.[11] Each mirror is placed in a 6 mm deep clearance hole in the spacer, drilled concentrically with the cavities. To allow for maintenance (exchange of mirrors), the mirrors were held in place by the use of O-rings, which,

[9] Primarily the diameter of the cavities, the thickness of the mirrors, and the distance between the cavities, the latter to assess the conditions under which there is a cross-talk between the different cavities bored in the same material.

[10] The use of Invar as the cavity spacer implies that the spacer could get a number of appealing properties for refractometry, e.g. that the cavity system could be made "*closed*" — which implies that the gas does not fill a volume surrounding the spacer as is the case for an "open" system (instead it fills only one of the cavities); that the cavities could be machined in a standard metal workshop whereby the cavities can be made with a *narrow bore* — which implies that each filling of gas brings in only a small volume of gas and thereby only a small amount of energy (when 100 kPa is addressed, < 0.5 J), minimizing any possible pV-work, and that the gas rapidly takes the temperature of the cavity wall (within a fraction of a second); that the spacer has a *high volumetric heat capacity* — which implies that a given amount of energy (supplied by the gas) only provides a small temperature increase in the spacer material; that the spacer has a *high thermal conductivity* and that the system could be constructed *without any heat islands* (i.e. regions that are connected with low thermal conductance) — which imply that any possible small temperature inhomogeneity created by the filling or evacuation of gas will rapidly spread in the system (significantly faster than in systems with cavity spacers made of glass materials, with larger gas volumes or with heat islands) so as to make the temperature of the DFPC-system homogeneous in a short time, which is a prerequisite for an accurate assessment of the temperature of the gas when using short modulation cycles; and that the spacer has a *low degree of He diffusivity and permeation*, significantly lower than that of ULE glass — which implies that there are virtually no memory effects when He is addressed.

[11] This reflectivity and mirror separation result in a finesse of 10^4 and, for the wavelength used, an FSR of 1 GHz.

in turn, were pressed in by two back plates, mounted on each side of the spacer [27].

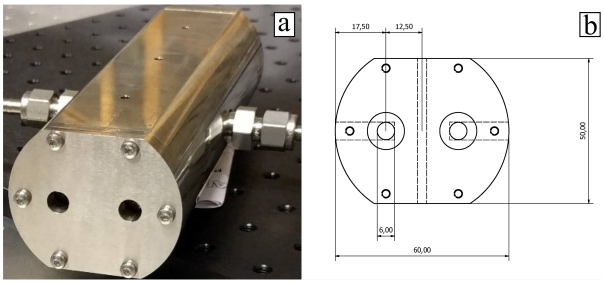

Figure 7. Panel (a): The Invar cavity assembly before being equipped with temperature probes and mounted inside the aluminium oven. The plates screwed into the spacer at its short ends press the mirrors, via O-rings, onto the spacer. Panel (b): A schematic drawing of the cavity assembly. Units in mm. Reproduced with permission from Ref. [32].

It is important to note that the mirror mounting differs markedly from that of optical contacting, which is commonly used and addressed in the other simulations. Since the mirrors, which are curved with a radius of 500 mm, are pressed onto the Invar spacer, only their outer rim will physically be in contact with and be pressed into the spacer by the compression of the O-rings. Moreover, since the limit of plastic deformation is lower for Invar than glass, the Invar spacer will plastically deform to form the contact surface between the mirror and spacer. An initial simulation was therefore performed to estimate the force by which each mirror is pushed into the spacer by the back plate which, in turn, determines the width of the contact rim. While the former was assessed to 69 N, the latter was estimated to be in the low µm range [33].

To assess the dominating parametric dependencies and to estimate the net deformation, simulations were performed, in the same manner as above, i.e. as a parametric study of the role of three parameters performed, in this case with regard to the cavity diameter, the rim width, and the cavity separation.

It was found, in contrast to the systems in which the mirrors are attached by optical contacting, that a change in cavity diameter of the bore in the Invar spacer does not change the area on which the gas is acting on the mirror; this is, in all cases, given by the area of the mirror within the rim. This implies that, in this cavity system, the deformation will be virtually independent of the cavity diameter [33].

It was instead found that the width of the rim (i.e. the width of the contact area between the mirrors and spacer) plays the main role in how much deformation the cavity experiences. A challenge for simulations is though that, since the contact area is small, its size and form will be affected by the roughness of the surface. Although the spacer surfaces have a non-negligible amount of roughness, the simulations assumed that the spacer surfaces did not have any roughness. This implies that it was difficult to, by use of simulations, accurately estimate the rim width. The simulations indicted though that, for a wide range of rim widths, ranging from 2 to 8 µm, the net pressure-normalized relative deformation of the two cavities, i.e. κ, will range from 7.8×10^{-12} Pa^{-1} to 6.7×10^{-12} Pa^{-1}, which correspond to a net refractivity-normalized relative difference in length, ε', ranging from 2.9×10^{-3} to 2.5×10^{-3}. It is surmised that the uncertainty in the contact area gives rise to the major part of the uncertainties in the simulations that, for the net pressure-normalized relative deformation, can be as large as 10^{-12} Pa^{-1}, and for the associated net pressure-normalized relative deformation, can be in the 10^{-4} range.[12]

All this indicates that it is not possible, by the use of simulations, to estimate the deformation of this system with such accuracy that it allows for assessments of pressure with the targeted uncertainty of 10 ppm. As is further discussed below, this system was therefore instead thoroughly characterized by the novel experimental characterization methodology developed.

3.4.2 Simulation of a closed single FPC system realized in a Zerodur spacer at PTB

PTB has simulated the pressure-induced deformation of a single closed FP cavity comprising a Zerodur-based spacer and two dichroic mirrors made from fused silica used at PTB. The 3D model is based, as realistically as possible, on the real system used at PTB. The spacer has a length of 100 mm, an

[12] This argument is also strengthened by a further analysis of the simulation, which shows that almost all deformation occurs in close proximity of the contact surface [33].

outer diameter of 40 mm, and a cavity bore diameter of 10 mm. The mirrors, which are glued to the spacer with Torr seal®, have a diameter of 15 mm and a thickness of 6.7 mm. The outer gas pressure was set to 100 kPa while the inner gas pressure was varied between 0 Pa and 100 kPa.

As is shown in Fig. 8, the simulations indicated that the pressure-normalized relative deformation of the Zerodur-based cavity, κ, is $2.6(1) \times 10^{-12}$ Pa^{-1}, which corresponds to a pressure-normalized relative deformation, ε', of $9.6(4) \times 10^{-4}$, where the uncertainties mainly originates from the glue.

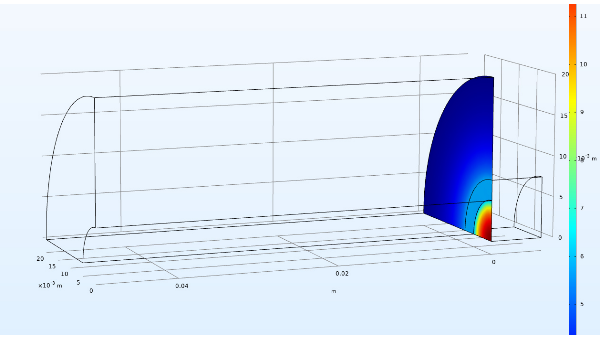

Figure 8. Pressure-normalized elongation of the dichroic Zerodur-based cavity system at PTB. It was found that the pressure-normalized relative elongation of the Zerodur-based cavity, κ, was $2.6(1) \times 10^{-12}$ Pa^{-1}

This implies that the uncertainties in the pressure- and refractivity-normalized relative deformations were estimated to 10×10^{-14} Pa^{-1} and 4×10^{-5}, respectively, which are a few times larger than the benchmarks (which are 2.7×10^{-14} Pa^{-1} and 1×10^{-5}, respectively). This implies that the simulation cannot assess the deformation with such a low uncertainty that it allows for an overall assessment of pressure of the targeted 10 ppm. The simulations can thus, in this case, solely be used as a rough estimation of the deformation; for a more precise assessment, another method must be used.

3.4.3 Simulations of a multi-cavity system based on sapphire components at PTB

PTB has also modeled a setup with one measurement cavity in the center and several reference cavities outside of the FP-spacer as is shown in Fig. 9.

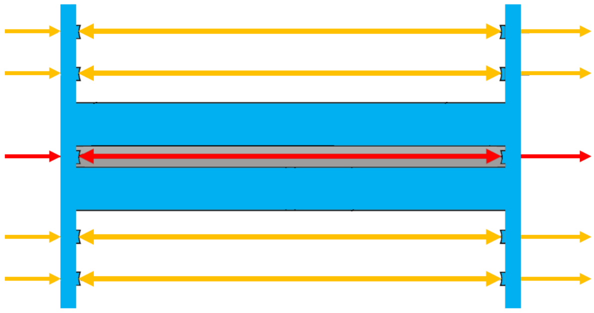

Figure 9. Scetch of the top view of the multi-cavity, as it is prepared at PTB. All parts are made from the same single crystalline type of sapphire with the same crystal orientation. White parts present the evacuated surroundings (outside) and the grey parts present the inner measurement chamber. This multi-cavity therefore has one closed measurement cavity (red beam) and four open reference cavities (orange beams).

Here, spacer, mirror substrates, and connectors were all made from sapphire. To match the real components fabricated at PTB in the simulations, the outer diameter of the spacer was chosen to be 37 mm and the diameter of the bore was set to 5.7 mm. The length of the spacer was taken as 100 mm. The mirror substrates have a thickness of 8 mm and a diameter of 50 mm. It was found that the net pressure-normalized relative deformation was one order of magnitude smaller than that for the Zerodur-based FP-cavity, viz. $2.0(2)\times10^{-13}$ Pa^{-1}, which corresponds to a refractivity-normalized relative deformation of $7.4(7) \times 10^{-5}$.[13] This implies that the relative uncertainties of the pressure- and refractivity-normalized relative deformations were estimated to be 2×10^{-14} Pa^{-1} and 0.7×10^{-5}, which again are within the 2.7×10^{-14} Pa^{-1} and 1×10^{-5} benchmarks.

However, it is worth to mention that, since the sapphire parts used for the components of this FP-cavity are of highest purity, mono-crystalline, and made from the same batch with the same crystal orientation, it can be assumed that gradients in the material parameters, i.e., the Young's modulus and the Poisson ratio, will be negligible. The compression of

[13] For a gas pressure of 100 kPa, this corresponds to an elongation of 2 nm of which 80% originated from the compression and deformation of the mirror substrates and 20 % from the elongation of the spacer itself, which thus also represents the elongation of the reference cavities.

the FP-cavity spacer can be directly assessed experimentally via the evacuated FP-cavity itself when the outer pressure is varied. This will potentially lead to much smaller uncertainties, presumably less than a percent.

Although this realization in principle could provide an assessment of the deformation that could contribute to the total uncertainty in a pressure assessment on a level below 10 ppm, it suffers from a few major challenges of which some are the assembly of the components by optical contacting and the associated geometrical uncertainties.

3.4.4 Simulation of an open single FPC system realized in a Zerodur spacer at CNAM

CNAM has modeled the deformation of a recently constructed open cavity bored in a Zerodur spacer with bonded silica mirrors. However, to optimize the design of the novel cavity spacer system, first the previous cavity system was analyzed by the use of simulations. For the design of the new FP-refractometer, both cylindrical and squared spacer blocks were considered and simulated. CNAM investigated, by the use of simulations by variation, the influence of the form of a Zerodur spacer with such shapes. These simulations led to the conclusion that the novel cavity system should be made in a 50 mm-squared block of Zerodur in which holes were bored according to Fig 10, viz. with two 12.5 mm diameter holes for the two mirrors, two 10 mm diameter holes for the gas filling, and two 10 mm radius holes for temperature measurements (as close as possible to the gas).

To simplify the modelling of this system, the cavity was considered to have flat mirrors mounted to the cavity spacer by optical contacting. As is shown in Fig. 11, the simulations indicated that the pressure-normalized relative deformation of the novel cavity, κ, is $-6.85(3) \times 10^{-12}$ Pa^{-1}, which corresponds to a refractivity-normalized relative deformation of $2.56(1) \times 10^{-3}$. This implies that the uncertainties in the pressure- and refractivity-normalized relative deformations, which were estimated to be 3×10^{-14} Pa^{-1} and 1.1×10^{-5}, respectively, are just above the corresponding 2.7×10^{-14} Pa^{-1} and 1×10^{-5} benchmarks.

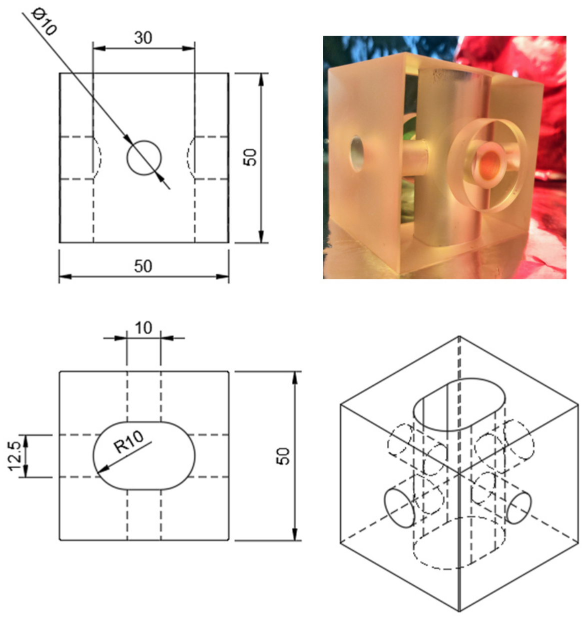

Figure 10. Drawing and picture of the novel CNAM FP-based cavity composed to a Zerodur 50 mm-squared spacer and two mirrors in fused silica mounted by optical contacting.

3.4.5 Simulation of a single FPC system at CEM

CEM has addressed the deformation of a single FPC system realized in Ohara's NEXCERA CD107 with mirrors made of ClearCeram-Z (CCZ) Regular.

NEXCERA™ is an ultra-low thermal expansion ceramic with a cordierite base (2MgO-2Al2O3-5SiO2). It has a number of properties that makes it appealing for FP-based refractometry, primarily the following ones:

1. It has a (near) zero thermal expansion coefficient at temperatures close to room temperature;
2. It has a high aging and thermal stability;
3. It has a high stiffness; about 50% higher than general low thermal expansion glass;
4. Since it is a pore-less material, it can be given a mirror finish by lapping and polishing; and
5. It can be sintered with near net shapes, enabling manufacturing of complex shapes at low cost.

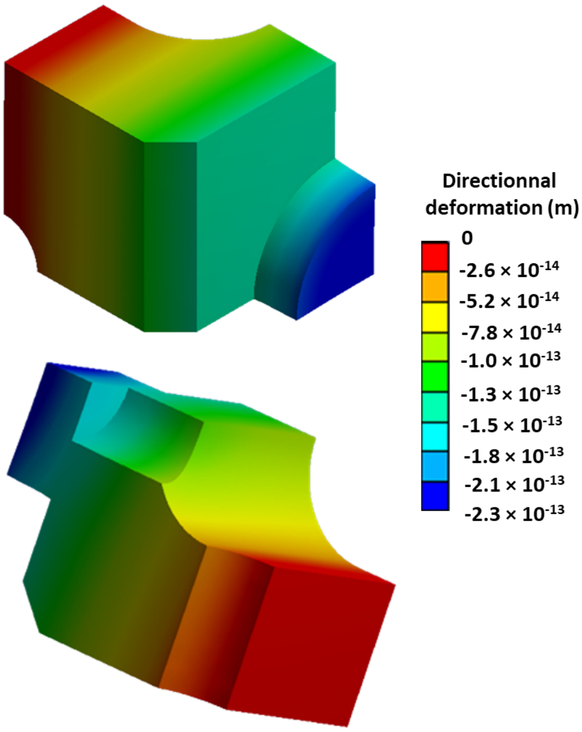

Figure 11. Cross section of the CNAM FP-cavity. The colour surface represents the directional deformation of the cavity material relative to the centre of the cavity. The simulations were performed with Ansys for a pressure of 1 Pa inside and outside the cavity.

Initially, a study of the optimum geometry of the spacer was made and, based on that geometry, a study of different materials was made. The final design is shown in Fig 12.

The deformation simulations were made under assumption that the cavity was made by Zerodur. The deformation was estimated by simulations at a set of pressures. The final value of the pressure-normalized relative deformation, which was assessed to -5.75(5) × 10^{-12} Pa^{-1}, which corresponds to a refractivity-normalized relative deformation of 2.15(2) × 10^{-3}, was achieved, by the use of the least squares method, as the slope of the plot. The uncertainty was estimated by a calculation of the covariance of the fitted parameters.

The analysis was carried out by simulating the absolute deformation of the mirror with an evacuated cavity exposed atmospheric pressure. The results of the mirror deformation for different mirror configurations are shown in Fig. 13 where R1 is mirror one and R2 is mirror 2. The light is introduced in the cavity though the R1 mirror, which implies that it needs a certain degree of transmission. The multiple reflections that take place between R2 and R1 gives rise to the various cavity modes.

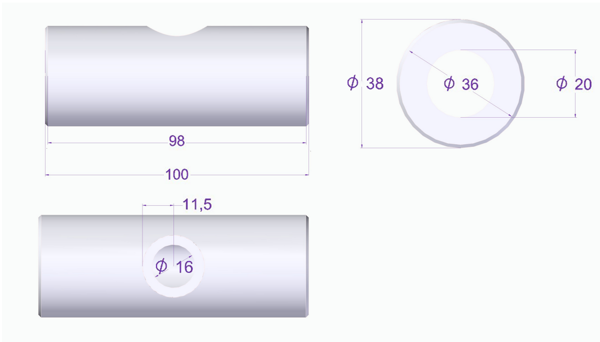

Figure 12. Cavity geometry of the FP system simulated by CEM. Dimensions are in mm.

Figure 13 shows that although the configuration of two mirrors made of NEXCERA has the lowest deformation, it was found that this configuration cannot be used as a FP-cavtiy since NEXCERA does not provide sufficient transmission of light. Under specific treatment it could be used as a highly reflective mirror but not as a mirror with adequate transmission. An working configuration could be made though by selecting R2 of NEXCERA and R1 made of anther material. Figure 13 shows that the configuration with R1 made of CCZ presents a lower deformation than the other configurations (Ultra Low Expansion Glass (ULE) and Zerodur 38 mm).

4 Experimental characterizations

Following the activity A1.1.3 in the "QuantumPascal" project, UmU, RISE, PTB, and CNAM then experimentally characterized one of their cavities with respect to its cavity deformation.

4.1 Development of a disturbance-resistant methodology for assessment of cavity deformation

Despite the fact that the two-gas method proposed by Egan et al. does not require accurate knowledge of the pressure — it is sufficient if it is con-

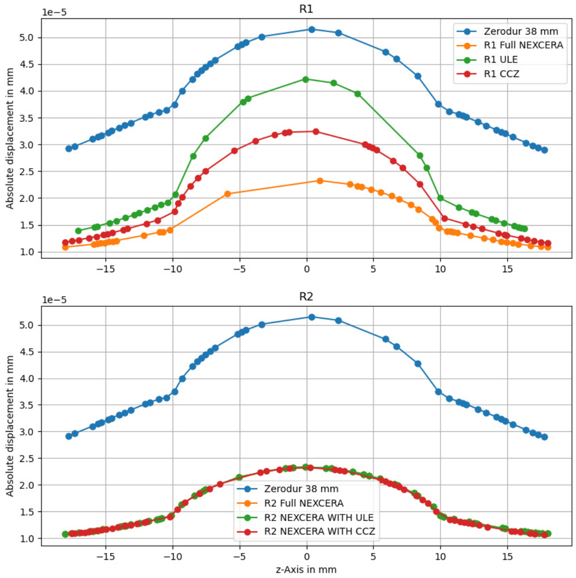

Figure 13. Simulations by CEM of mirror deformations for different mirror configurations.

stant [21] — it potentially opens up for influence of disturbances from a number of physical processes, e.g. drifts, gas leakages, and outgassing, that can deteriorate the uncertainty of the assessed cavity deformation.

To mitigate the influence of such disturbances, Zakrisson et al. developed, within the "QuantumPascal" project, a robust and disturbance-resistant method for assessment of deformation that is not affected to the same extent of these types of disturbances [22]. It is based on scrutinizing the difference between two pressures — one provided by an external pressure reference system (in this case a pressure balance, RUSKA) and the other being the pressure assessed by the refractometer — as a function of pressure (i.e. for a series of (set) pressures), evaluating the data by use of a model that does not incorporate cavity deformation, for two gases with dissimilar refractivity, He and N_2. For best performance, the methodology was carried out by use of the GAMOR methodology. By fitting linear functions to the pressure-dependent responses and extracting their slopes, the cavity deformation caused by pressurization could be obtained with high accuracy (primarily with a reduced influence of gas leakages and outgassing) in term of the pressure-normalized relative deformation, ε' [22].

A thorough mathematical description of the procedure served as a basis for an evaluation of the basic properties and features of the procedure. This indicated that the cavity deformation assessment is independent of systematic pressure-independent (constant) errors in both the reference pressure and the assessment of gas temperature. In addition, since the GAMOR methodology is used, the assessment is immune to linear drifts [34] and has an additional reduced sensitivity to gas leakages and outgassing into the system. Thus, the methodology developed provided a robust assessment of cavity deformation with small amounts of uncertainties [22].

As is further discussed below, it was concluded that when a high-precision (sub-ppm) refractometer (which often can be obtained when the GAMOR methodology is used) is characterized by this methodology, and under the condition that high purity gases are used, assessment of the deformation could be made with such small uncertainty that it solely contributes to the uncertainty in the assessment of pressure of N_2 to a level of 1 or 2 ppm (depending on which type of N_2 pressure standard it refers to; a mechanical or a thermodynamic one, respectively) [29]. This implies, in practice, that, as long as gas purity can be sustained, cavity deformation is no longer a limiting factor in FP-based refractometer assessments of pressure of nitrogen.

4.2 Experimental characterization of Invar-based DFPC refractometers by UmU and RISE

The Invar spacer scrutinized in Section 3.4.1.2 above was used in the realization of two FP-based refractometer systems, one at UmU, referred to as the Stationary Optical Pascal (SOP) [27–29, 31, 32], and one at RISE, denoted the Transportable Optical Pascal (TOP) [29–32, 35].

4.2.1 Experimental characterization of the stationary Invar-based DFPC refractometer (the SOP) at UmU

In a first assessment of the net pressure-normalized relative deformation of the SOP, i.e. κ, performed at the time for the development of the novel characterization method, it was found that it could be assessed, for pressures up to 16 kPa, under the condition that the gases do not contain any impurities, when the molar polarizability of N_2 was traced to a mechanical pressure standard, with a relative uncertainty of 0.2% to $5.258(6) \times 10^{-12}$ Pa^{-1}, which corresponds to a net pressure-normalized relative deformation, ε', of $1.963(2) \times 10^{-3}$ [22].[14]

At a later instant, however, when the SOP had been refurbished and upgraded, it was found that the deformation was slightly dissimilar, viz. $1.972(1) \times 10^{-3}$ [29]. It should be noted though that in between these two assessments, the mirrors of the two cavities in the SOP system had been de- and remounted for maintenance purposes. Although not yet confirmed, the alteration in deformation of the SOP system between these two instants can be attributed to either this procedure or, alternatively, impurities in the He.

It is also worth to note that, as a consequence of the upgrade of the SOP system, the assessment of the refractivity-normalized relative deformation could be made with an improved uncertainty, viz. 1×10^{-6}. Since this uncertainty contributes to the uncertainty in the assessment of pressure with 1 ppm, and since this presently solely is a fraction of the uncertainty of the molar polarizability of nitrogen, this implies that, in practice, as long as gas purity can be sustained, cavity deformation is no longer a limiting factor in FP-based refractometer assessments of pressure of nitrogen.

It should also be noticed that these deformation values differ markedly from the simulated ones (as given in section 3.4.1.2); they are orders of magnitude better. As was alluded to above, the main reason for this is attributed to a difficulty in the simulations to properly assess the shape and minuscule size of the contact area between the curved mirror and the spacer. As is shown above though, this does though not hamper an experimental assessment of the deformation to a level well below the benchmark that represents an uncertainty of a pressure assessment of 10 ppm.

4.2.2 Experimental characterization of the transportable Invar-based DFPC refractometer (the TOP) at RISE

At the same time as the deformation of the SOP was assessed the second time, also the deformation of the TOP at RISE was assessed. Although the design of the two systems is identical, it was found that ε' of the TOP differed from that of the SOP by 2.3%; it was found to be $1.927(1) \times 10^{-3}$, thus with an uncertainty of likewise 1×10^{-6}, well below the benchmark [29].[15]

Furthermore, UmU and RISE also made a preliminary characterization of the TOP with regard to its deformation for pressures up to 100 kPa by the use of a traceable pressure balance at RISE (Ruska 2365A-754) [30, 35]. To reduce the risk for drift-induced errors, measurements were performed at nine different pressures in randomized order. The data were evaluated using standard expressions for refractivity, molar density, and pressure in the absence of cavity deformation (and, for simplicity, neglecting any possible influence of mirror penetration depth and Gouy phase) [23], i.e. by use of the Eqs. (1b) and (4) in Zakrisson et al. [22] with both the relative deformation and the mirror penetration depth set to zero.

Although the response of this characterization was looking ostensibly linear on a pressure-of-the-TOP-vs-set-pressure plot, it was found that the response was weakly non-linear. A fit to the data provided a response of the refractometer of the form $(a + bP + cP^2)$, where $a = -0.614$ Pa, $b = 1.0021$, and $c = 1.52 \times 10^{-9}$ Pa^{-1} [35].

The deviation of the b parameter from unity was mainly attributed to the fact that the refractometer was evaluated with the deformation parameter set to 0. Likewise, the non-linearity was attributed to a weak second order pressure dependence of the relative deformation, $\Delta L/L$, possibly caused by the particular mirror mounting or the mirrors (in which the rim of the mirror is pressed into the cavity spacer material so as to plastically deform some part of the spacer) [35]. This non-linearity has not clearly been seen before, when only pressures up to a few tens of kPa were addressed, as was the case in [29] and [22]. This feature will be addressed in a future work.

[14] For the case when the molar polarizability of N_2 was traced to a thermodynamic pressure standard, the corresponding values became $5.258(12) \times 10^{-12}$ and $1.963(4) \times 10^{-3}$, respectively.

[15] It is not yet assessed whether this difference between the two Invar-based systems is within the expected variation of deformation of two systems comprising the particular "press-on" mirror mounting used in the SOP and the TOP or whether it should be attributed to the mirror de- and remounting process that was carried out in one of the systems. Work aimed at further investigating this will be pursued in the closest future.

4.3 Experimental characterization of a Zerodur-based single FP cavity refractometer by PTB

PTB has experimentally characterized the pressure induced deformation of the single Zerodur-spacer-based FP-cavity utilizing mirrors based on fused silica fixed by resin glue (Torr seal®) that was simulated above, utilizing the two-gas method with He and N_2 developed by [22]. For this purpose, different gas pressures were realized at a constant temperature of 23.256(10) °C. The reference pressure sensors (type Mensor 'CPT9000') were calibrated directly in PTB's vacuum laboratory. Also, an additionally reference pressure was realized by a pressure balance at 29.15 kPa. For nitrogen 13 pressure points and for helium 11 pressure points in the range of 100 Pa to 100 kPa have been assessed. The experimentally determined refractivity-normalized pressure-induced relative deformation, ε', was determined to $1.0(2)\times10^{-3}$, where the uncertainty represents one standard deviation.

4.4 Experimental characterization of a Zerodur-based single FPC refractometer by CNAM

CNAM has initiated a characterization of their new Zerodur-based single FP cavity refractometer with respect to its pressure-induced cavity deformation up 100 kPa by the use of LNE's pressure balance reference (DHI PG 7607, 20 cm^2 piston cylinder), which has a $k = 2$ uncertainty of 0.20 Pa $+9\times10^{-6}P$.

So far, only a first preliminary characterization of the deformation of the FP-cavity has been carried out. Since only a single cavity was used, and since, in this first characterization, the two-gas method was not utilized to eliminate ageing and drifts, different cycles between vacuum (our reference) and gas pressure up to 100 kPa in N_2 were performed during one day. To minimize temperature effects during cycles, and to avoid corrections due to thermal expansion, the FP-based cavity was regulated to the gallium melting point with a stability of ca. 1 mK. Based on assessments of the beat frequencies in vacuum and with gas present, which were assessed with a standard deviation of 300 Hz and 8 kHz, respectively, the free spectral range (assessed to 2997812.6 kHz), which could be assessed with a standard deviation of 1.8 kHz, and the temperature of the gas, which could be assessed with a standard deviation below 1 mK, it was possible, by use of standard expressions for refractivity and molar density in the absence of cavity deformation, to perform a preliminary assessment of the pressure-normalized relative deformation, κ. This was assessed to -6.70(2) × 10^{-12} Pa^{-1}, which differs from the simulated value solely by 2 %. This implies that the pressure-normalized relative deformation so far has been estimated with an uncertainty of 2×10^{-14} Pa^{-1}, which is a sightly smaller than the 2.7×10^{-14} Pa^{-1} benchmark.[16]

4.5 Experimental characterization of a single FPC system realized in a NEXCERA spacer at CEM

CEM is presently in the process of finishing the assembly of their experimental system. Results of this task will therefore be obtained when this is completed.

5 Conclusions

Since pressure-induced cavity deformation affects assessments of refractivity (and thereby pressure), to be able to utilize FP-based refractometry for assessment of pressure, or as standards, this concept has to be adequately addressed. There are two ways this can be done; either by the construction of systems with no (or virtually no) cavity deformation, or by an accurate characterization of systems with finite amounts of deformation.

Although it is possible in theory to construct FP-cavities that have virtually no net deformation, it was, in this project, soon concluded that such designs need to be rather complex, wherefore they cannot be implemented at a reasonable cost due to the prevailing manufacturing tolerances.

The work within the addressed Task 1.1 of the "QuantumPascal" project was therefore mainly devoted to characterizations of various types of FP-based refractometers, either by simulations or by experimental means.

The work in this Task was carried out in the following way. After a general parametric study of a

[16]For a full characterization of the system, i.e. to complement the preliminary assessment, additionally work needs to be done, among other things, a characterization based on the two-gas method. Work along these lines will be pursued in the closest future.

single closed cavity with mirrors firmly attached to the spacer by simulations based on finite element methods (FEM), several existing FP-cavity systems were characterized with respect to their pressure-induced deformation by the use of simulations. After this, a number of existing systems were characterized with respect to their deformation by the use of experimental means.

5.1 Parametric investigation of the pressure-induced deformation of a FP-cavity

For the case with a single closed cavity with mirrors firmly attached to the spacer, a general parametric study, comprising a set of simulations presented in section 3.2, assessed the main dependencies of the most important parameters on the pressure-induced deformation. It was found that the deformation mainly has a quadratic dependence on the radius of the measurement cavity, a strong dependence on the thickness of the mirrors for mirror thickness smaller than the diameter of the cavity but a weak one for thickness larger than the bore, and, for all but the shortest cavity lengths, a proportional dependence on the length of the cavity.

For the case with mirrors pressed into the spacer material, which so far has been the case for the Invar-based system at UmU and at RISE, it was found, as is discussed in section 3.4.1.2, since the gas exerts pressure on the mirrors on the entire area within the rim of the mirror, that the deformation is virtually independent of the cavity diameter.

5.2 Simulations of a selection of FPC-systems

Four partners of the "QuantumPascal" project were simulating different types of cavities with varying geometries made from the presently most commonly used spacer materials, sapphire (1 system), Zerodur (4 systems), and Invar (1 system), with various mirror substrates and mountings, for both open and closed systems, representing cavity systems in which experimental characterizations were subsequently performed (or were planned to be performed).

5.2.1 Deformations assessed by simulations

It was found that the net pressure-normalized relative deformations ranged from $0.20(2) \times 10^{-12}$ Pa^{-1}, which was achieved for the closed multi-cavity system based on sapphire components at PTB, via $0.76(2) \times 10^{-12}$ Pa^{-1}, which was obtained for the closed DFPC system realized in a Zerodur spacer with mirrors mounted by optical contacting at UmU, $2.6(1) \times 10^{-12}$ Pa^{-1}, which was obtained for the closed single FPC system realized in a Zerodur spacer with mirrors mounted by glue at PTB, and $-5.75(5) \times 10^{-12}$ Pa^{-1} , which was obtained for the single FPC system realized in a Zerodur spacer at CEM, up to $-6.85(3) \times 10^{-12}$ Pa^{-1}, which was obtained for the open single FPC system realized in a Zerodur spacer at CNAM, and to values in the 6.7×10^{-12} Pa^{-1} to 7.8×10^{-12} Pa^{-1} range for the closed DFPC systems realized in Invar spacers at UmU and RISE. This implies that the amount of deformation of the systems addressed differ roughly by a factor of 35.

The corresponding values of the pressure-normalized relative deformations ranged similarly from 75×10^{-6} to 2900×10^{-6}. This implies that cavity deformation contributes to the assessment of refractivity (and thereby pressure) on a level ranging from 75 ppm to 2.9 ‰.

The reason for this spread in deformation is that the systems are configured dissimilarly. Although there, in general, are several differences between the systems, it is though often possible to identify the generally dominating causes for the pertinent level of distortion.

The smallest deformation was obtained for the sapphire system. This originates mainly from the fact that sapphire has an exceptionally large Young's modulus. The deformation in this system was found to be about a third of a that of the DPFC Zerodur based system realized at UmU. This Zerodur based system was, in turn, found to have about a third of the deformation of the DFPC system based on Zerodur at PTB. The reason for this was attributed to the fact that the former was considering a system with mirrors mounted by optical contacting, while the latter one utilized glue. The latter one was again found to have almost a third of the deformation of the single FPC system realized in a Zerodur spacer at CEM and a third of the deformation of the open single cavity system based on Zerodur at CNAM. The reason for this is attributed to the fact that while the PTB system was a closed one, the CEM and the CNAM systems were open, which implies that the gas pressure could act on the entire short-end of the cavity spacer (and not only on the part of the mirror to which the gas in the cavity is exposed).[17] It could finally be concluded that although the closed Invar-based systems at UmU and RISE were realized with a narrow cavity bore, the pressure-induced deformation was considerable, of similar magnitude to that of the open system realized in Zerodur by CNAM. The reason to this was attributed to fact that for the mirror mounting utilized in the Invar system, the gas exerts pressure on the mirrors on the entire area within the rim of the mirror.

5.2.2 Uncertainties in the simulated amounts of distortions

Although it is advisory to realize and utilize systems that have small amounts of deformation, not all systems with small deformation provide the most advantageous conditions. Those are instead produced by the systems whose deformation can be assessed with the smallest uncertainty. It was concluded in section 2.2 above that the (absolute) uncertainty in the assessed pressure-normalized relative deformation, i.e. $\delta\varepsilon'$, represents the relative contribution to the uncertainty of the overall pressure assessment from the deformation, i.e. $\delta P/P$.

Based on the 1×10^{-5} benchmark for the uncertainty of ε', it could be concluded that two of the simulations could provide deformations with uncertainties that are below this benchmark, viz. the multi-cavity sapphire system at PTB and the DFPC Zerodur system at UmU, which ended with uncertainties in ε' of 0.7×10^{-5}, while one, the Zerodur spacer system at CNAM, provided a deformation whose uncertainty was more or less equal to the benchmarks (with an uncertainty in ε' of 1.1×10^{-5}).

The simulation of the Zerodur-based system at CEM provided an uncertainty that was twice the benchmark, while the Zerodur system at PTB, which incorporated glued mirrors, provided an uncertainty that was four times the benchmark. The reason for the latter was mainly attributed to glue used for the mounting of the mirrors.

The simulations for the Invar system, which suffers from a poor modelling of the mirror mounting, in turn, ended up with one order of magnitude larger uncertainty than the glued Zerodur system at PTB. This was mainly attributed to the uncertainty in the geometrical parameters of the spacer-to-mirror interface (the rim) caused by a difficulty to, in the presence of the pertinent surface roughness, sufficiently accurately model and assess the plastic deformation of the spacer material.

In summary, it was thus found that, although it is possible to model most types of system by the use of simulation programs, the accuracy by which the simulations can predict the deformation is often either marginally sufficient or insufficient to allow for assessment of pressure with an overall uncertainty of 10 ppm. The simulations are either limited by the uncertainty in the material parameters used, e.g. the Young's modulus and the Poisson ratio, which often are in the percent to permille range, or by the ability to model the system appropriately in the simulation program. The latter is particularly the case for systems with mirrors mounted to metal spacers by a press-on approach that provides plastic deformation of the spacer or those utilizing glue for the mounting of the mirrors. This implies that it is not suitable to rely on simulations for assessing the deformation of such systems.

It can also be concluded that, for the other types of system, a deformation-characterization based solely on simulations will only seldom, preferably when the deformation is small, and then presumably only barely, provide characterizations that allow for assessments of pressures with the targeted relative uncertainty of 10 ppm.

5.3 Experimental characterizations of existing FPC-systems

Over the years, a number of experimental characterization methodologies have been proposed. One such approach was suggested and scrutinized by Ricker et al. [25] and Takei et al. [26]; by comparing multiple systems with dissimilar lengths, or changing the length of a system with adjustable length, it should, at least in principle, be possible to separately assess pressure-induced deformations of the cavity spacer and the mirrors. However, it was found that the accuracy of this type of assessments is limited, mainly

[17] It was concluded that that a cavity made of Ohara's NEXCERA with CCZ Regular mirrors and a cylindrical shape can reduce the deformation with respect some other configurations of shapes and materials, in particular Zerodur.

by mechanical stability and stringent manufacturing tolerances. This implies that this methodology should be exercised with caution.

Alternative means to assess the deformation, e.g. those proposed by Stone and Stejskal [11] and by Egan and Stone [21], comprise the use of two gases with dissimilar refractivity, so as to cancel the deformation or to either assess the change in refractivity when one gas is replaced by another or evaluate two such assessments by a methodology that allows for an unequivocal assessment of the deformation. Although these types of methodology are useful for well-stabilized systems, they are in practice often affected by, and sometime even restricted by, various types of external disturbances, e.g. drifts in the cavity length, the reference pressure, or the temperature, gas leakages, or outgassing.

As a means to mitigate the influence of such disturbances, a novel robust methodology has been developed that allows for assessments of cavity deformation that are independent of systematic pressure-independent (constant) errors in both the reference pressure and the assessment of gas temperature, and, when carried out by use of the gas modulation refractivity (GAMOR) methodology, is additionally insensitive to gas leakages and outgassing, and immune to linear drifts (e.g. in the cavity length) [22].

5.3.1 Experimentally assessed distortion of the Invar-based DFPC systems at UmU and RISE

This methodology was applied to the assessment of deformation, first in the stationary Invar-based DFPC refractometer at UmU (the SOP), and later also in the TOP system at RISE. It could be concluded that this procedure provided deformation values with significantly lower uncertainty than the simulated ones; while the simulations provided pressure-normalized relative deformations ranging from 7.8×10^{-12} Pa^{-1} to 6.7×10^{-12} Pa^{-1}, which correspond to a refractivity-normalized relative deformation, ε', in the 2.9×10^{-3} to 2.5×10^{-3} range [33], the experimental assessment of the deformation in the SOP system provided, for pressures up to 16 kPa, a pressure-normalized relative deformation of $5.258(12) \times 10^{-12}$ Pa^{-1}, which corresponds to a refractivity-normalized relative deformation of $1.963(4) \times 10^{-3}$ [22].

At a later instant, however, when the SOP was characterized with respect to its total uncertainty, it was found that the deformation was slightly different, viz. $1.972(1) \times 10^{-3}$ [29]. Although not yet confirmed, the change in deformation between these two instants was attributed to either the remounting of the cavity mirrors or contamination of the He gas.

Regarding the transportable Invar-based system at RISE (the TOP), the same experimental characterization provided, for pressures up to 16 kPa, a refractivity-normalized cavity deformation of $1.927(1) \times 10^{-3}$.

It has thus been found that, despite the slightly dissimilar values of the assessed pressure-induced cavity distortion of the SOP and the TOP,[18] their uncertainties, which thus both were 1×10^{-6}, were found to be significantly below the benchmark. This implies that when the systems are otherwise well-characterized, these deformation assessments are accurate enough to allow for assessments of pressure well within the targeted relative uncertainty of 10 ppm.

5.3.2 Experimentally assessed distortion of the Zerodur-based single FPC system at PTB

PTB has experimentally characterized (via the two-gas method with He and N_2) the pressure induced deformation of the single cavity Zerodur-based FP-system utilizing mirrors based on fused silica fixed by resin glue (Torr seal®). It was found that the experimentally assessed refractivity-normalized cavity deformation agrees with the simulated one within their uncertainties: $\varepsilon'_{experiment} = 1.0(2) \times 10^{-3}$ and $\varepsilon'_{simulation} = 9.6(4) \times 10^{-4}$, respectively.

This implies that it could be concluded that, due to the use of the resin glue, the pressure-induced elongation of this cavity is considerable. It could also be concluded that its uncertainty is above the benchmark. Therefore, this cavity is not suitable as a basis for the realization of a primary standard. Instead, it

[18] It is relevant to point out though that although the cavity design and construction of the SOP and the TOP are virtually identical, the experimentally assessed deformations still differ outside their uncertainties. As was alluded to above, the cause of this has been attributed to the unconventional mirror-mounting, which, to provide a good seal, incorporate a plastic deformation of parts of the Invar spacer. Although this might be a sturdy and well working mirror mounting for any given system, this clearly demonstrates the need of experimental assessment of the deformation (rather than assessment by simulations).

will henceforth mainly be used as a stable evacuated reference cavity for beat measurements at 633 nm and 1550 nm.

5.3.3 Experimentally assessed distortion of the new Zerodur-based single FPC refractometer at CNAM

The new Zerodur-based single FP cavity refractometer at CNAM has been subjected to a first preliminary characterization of the deformation. In this, the pressure-normalized relative deformation, κ, was assessed to $-6.70(2) \times 10^{-12}$ Pa^{-1}, which differs from the simulated value solely by 2 %. This implies that the pressure-normalized relative deformation so far has been experimentally estimated with an uncertainty of 2×10^{-14} Pa^{-1}, which is a sightly smaller than the 2.7×10^{-14} Pa^{-1} benchmark.[19]

5.3.4 Experimentally assessed distortion of the transportable system used for the ring comparison up to 100 kPa at RISE

Finally, when the RISE transportable system, as a part of the ring comparison performed within work package 4 of the "QuantumPascal" project, was compared to a pressure balance at pressures up to 100 kPa, it was concluded that, for higher pressure, a deviation from a linear dependence of the pressure-induced cavity deformation could be seen [35], the origin of which is subjected to further investigation.

5.3.5 Experimentally assessed distortion of an FPC system realized in a NEXCERA spacer at CEM

Since CEM presently is in the process of finishing the assembly of the experiment, results from their experimental characterization will be obtained when this is completed.

5.4 Conclusive remarks

It was concluded from the simulations presented above that the accuracy by which the simulations can predict the deformation is often either marginally sufficient or insufficient to allow for assessment of pressure with an overall uncertainty of 10 ppm. The simulations are either limited by the uncertainty in the material parameters used, e.g. the Young's modulus and the Poisson ratio, which often are in the percent to permille range, or by the ability to model the system appropriately in the simulation program.

On the other hand, it was demonstrated that pressure-induced distortion can be assessed by experimental means with an uncertainty well within the benchmark, in particular if the novel methodology for assessment of pressure-induced distortion that provides assessments that are independent of systematic pressure-independent errors in both the reference pressure and the assessment of gas temperature, and, when carried out by use of the gas modulation refractivity (GAMOR) methodology, also is insensitive to gas leakages and outgassing, is used. It was demonstrated that when a high-precision (sub-ppm) refractometer is characterized according to this methodology, and when high purity gases are used, the uncertainty in the deformation solely contributed to the uncertainty in the assessment of pressure of N_2 with 1 ppm, thus allowing refractometry to be assessed in an otherwise well-characterized system well within the 10 ppm targeted uncertainty. This methodology was, in this project, applied to the assessment of deformation in several FPC systems.

As has been demonstrated by CNAM, also conventional refractometry (i.e. refractometry not utilizing the GAMOR methodology) has been used to experimentally assess pressure-induced distortion to within the benchmark.

6 Recommendations

All FP-based refractometry systems must, unless they are calibrated towards some other pressure standard, and in particular if they are going to be used as an internal standard, be characterized with respect to their pressure-induced deformation. To reduce the required accuracy by which such a characterization needs to be done, it is advisory to realize a system with a minimum of pressure-induced deformations.

It has been concluded that means to construct FPC-based refractometry systems with small amounts of deformation preferably should include the following concepts:

[19] It is also pointed out though that, for a full characterization of the system, additional work is needed to complement the preliminary assessment. Work along these lines will be pursued in the closest future.

1. The use of a "closed cavity";[20]
2. For a closed cavity: the use of a small diameter for the cavity bore;[21]
3. The use of a spacer material made of a stiff material (i.e. a large Young's modulus);[22]
4. The use of a mirror substrate made of a stiff material (i.e. a large Young's modulus),[23] whose thickness is at least as large as the diameter of the cavity bore;
5. Avoid using glue for mirror mounting and, when appropriate, use a sufficiently large contact area between the mirror and the substrate;[24]

It is not always possible to construct an FP-based refractometry system that fulfills all the points above. It is, in general, often necessary to balance the advantage of each of the points above with other aspects one has to consider when constructing a system (e.g. regarding the ability to assess the temperature and its susceptibility of pV-work).

Since, in the end, it is of highest importance that the pressure-induced deformation can be assessed with sufficiently low uncertainty, it can be concluded that although simulations often are considered to be a useful tool, it is not always possible to assess the cavity deformation with the required uncertainty by the use of simulations. For the case when the deformation is small enough, when the system can be modelled with sufficient accuracy, and when the system parameters can be retrieved with sufficiently low uncertainties, simulations are a possible means.

For some systems though, primarily the Invar-based DFPC developed and utilized by UmU and RISE, because of the particular mirror mounting in which the rim of the mirror is pressed into the cavity spacer material so as to, by plastic deformation of the spacer material, form a thin seal, it is not recommended to rely on simulations for assessment of the cavity deformation.[25] It is also questionable if simulations are suitable for systems in which the mirrors are mounted by the use of glue.

It is instead recommended that all systems should be characterized with respect to their pressure-induced deformation by use of an experimental means. When such characterizations are to be done, it is recommended to utilize, if possible, the methodology developed by Zakrisson et al. [22], since it makes the assessments immune to linear drifts and provides a significantly reduced sensitivity to gas leakages and outgassing in the system. The system has demonstrated assessment of cavity deformation with uncertainties that are one order of magnitude below the benchmark for making pressure assessment with 10 ppm uncertainty possible (i.e. with uncertainties in the ε' entity of 1×10^{-6}), which corresponds to a net pressure-normalized relative difference in length, 0.3×10^{-14} Pa^{-1} [29].

Finally, since He has such a distinct refractivity, any contamination in the gas will have an adverse effect on the assessment of the cavity deformation. A remaining issue regarding the use of an experimental characterization that utilizes He as one of the gases is therefore how to find means to minimize the potential contamination of the gas. Alternatively, it would be beneficial to investigate the possibility to develop and realize an experimental characterization methodology that does not rely on this gas.

[20] The concept of "closed cavity" refers to a system that solely fills the interior of the cavity with gas. The justification for this is that the force exerted by the gas on a piece of material is proportional to both the pressure and the area. Since the internal bore of a cavity is smaller than the "short ends" of a cavity spacer, the deformation of the cavity is in general smaller for a "closed cavity" system than an "open cavity" one (i.e. one in which the gas is applied to both the cavity and its surrounding).

[21] As is shown by Fig. 2, since the force by which the gas acts on a mirror is proportional to the area of the cavity bore, the use of a small diameter cavity will, when a "closed cavity" is used, provide a small force on the mirror, which leads to a small deformation.

[22] Since the deformation of a material depends on its stiffness, the use of a material with a large Young's modulus will, for a given force applied by the gas, give rise to a small cavity deformation.

[23] Similar to above, since the deformation of a material depends on its stiffness, the use of a mirror substrate with a large Young's modulus will, for a given force applied by the gas, give rise to a small mirror deformation and thereby a small cavity deformation.

[24] To reduce mirror deformation, it is advisory to avoid the use of small contact areas between the mirror and the cavity spacer.

[25] This does not mean that it is not recommended to use an Invar spacer in FP refractometers; on the contrary, due to all its appealing features (see above), it is still an experimental realization that should be considered of great interest for the realization of low-uncertainty refractometers. If an Invar-based refractometry system in which there is a larger concordance between simulations and experimental assessments is to be realized, a possible alteration of the Invar-spacer concept is to utilize an alternative type of mirror-mounting, e.g. one comprising metal gaskets for which the contact areas between the mirror and the cavity spacer is larger and no plastic deformation of the spacer takes place.

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