

VOL. 55, 2016



Guest Editors:Tichun Wang, Hongyang Zhang, Lei Tian Copyright © 2016, AIDIC Servizi S.r.I., ISBN978-88-95608-46-4; ISSN 2283-9216

Analysis of Misalignment Sensitivity of Generalized Ring Resonator for the Trace Gas Concentration Detection Instrument Based on CRDS

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Cavity Ring-Down Spectrometer (CRDS) (Romanini et al., 1997) has been widely used in the fields of atmospheric chemistry, meteorology, air pollution and greenhouse gas emission, ecological environment and ecological hydrology research and public safety assurance. However, in order to maximize the measurement sensitivity of the target analyte of the cavity ring down spectrometer, the absorption measurement should be selected at the target line absorption peak (Kevin K. Lehmann et al., 1996). In addition, it should be noted that the interference of absorption lines of the same or other species should be reduced, in order to achieve a higher accuracy detection of the instrument that improving the spectral accuracy become more critical (Altshuler et al., 1977). In the paper, we have considered the existence of the self-conjugate rays in the resonator which is consisted of a number of mirrors and including spherical mirrors, the effect of spherical mirror misalignment in ring resonators was investigated. Then by utilizing the optical path turning reflection matrix, and the influence that caused by both the displacements of a spherical mirror and plane mirror in a nonplanar ring resonator have been obtained, and given the relation of the error transmission in both azimuth and pitch direction.

1. Introduction

CRDS is a technological breakthrough of instrument in ultra-trace gas concentration detection, it provides high performance price ratio and more suitable for harsh site application conditions of the general gas detection means, while other existing test methods can not be compared with. CRDS is the only mean that achieve the real-time detection of CH₄, N₂O and other trace of greenhouse gases (Mikhailenko et al., 2005; Ma, 2016). CRDS is a mean for on-line monitoring of the highest sensitivity of trace water, hydrogen and oxygen isotope at present. In the field of volatile organic compounds, explosives and drugs harm public safety material (Risby et al., 2006), CRDS provides ultra high sensitivity, long stability and real-time that other means do not have. CRDS can be used as the standard configuration of gas analysis in analytical chemistry laboratory, the price cost of the whole set of instrument is equivalent to the most commonly used meteorological instrument Gas Chromatograph (GC) in the laboratory, but the sensitivity of CRDS is 10 to 10³ higher than that of GC. CRDS has the stability that the other trace analytical methods can not be compared with. CRDS technique can directly measure the isotopic content in water samples without pretreatment, and the sensitivity and stability can reach the $\delta^{18}O<0.1^{\circ}/_{.00}$, $\Delta d<0.5^{\circ}/_{.00}$, superior to the isotope ratio mass spectrometer (IRMS) that demanding laboratory operating conditions and sample pretreatment program. At present, the detection system based on non-straight cavity is widely used in many fields, such as gas spectral measurement and trace gas concentration detection. In 2002, Baer et al., Used the CRDS technique to measure the concentration of NH₃, CH₄, C₂H₂ and CO in atmosphere and mixed gas, and obtained the detection system sensitivity of 3.1×10⁻ ¹¹cm⁻¹Hz^{1/2}. In addition, the United States LRG company also began to provide the type of commercial gas detection and analyzer, depending on the object of its measurement accuracy order of magnitude up ppm to ppb. In 2012, Andreas and Rao Gottipaty established off axis CRDS measurement system.

169

2. Analysis method

CRDS is spectrum measurement technology based on the high quality passive cavity, the cavity is usually composed of two or more mirrors. Let the light be incident to a stable resonator, if it coincides with itself after a reflection by all the resonator mirrors, Thus, the optical axis of the resonator is closed, and will be called self-conjugate axis, the analysis of the existence and the characteristics of self-conjugate ray in a ring resonator converts to the identification of the axes in space whose image coincides with the axes selves after passing through all mirrors, and the all of self-conjugate rays compose a nonplanar surface which will be called the resonance surface of resonator.

We suppose the optical system is composed of N plane mirrors (M_1 , M_2 , ..., M_N) at any position. A righthanded coordinate system O_0 - $X_0Y_0Z_0$ is set up in the entrance mirror P_1 , Let the object point P_1 locate in front of the mirror M_1 . The construction of an image generated by an arbitrary mirror M_J can be described by a reflection operator \hat{P} relative to the plane coinciding with the mirror.



Figure 1(a): Right-handed coordinate systems; Figure 1(b): A self-conjugate ray of nonplanar resonator with an even number of mirrors;

Then, the system $O_n - X_n Y_n Z_n$ is obtained from the system $O_0 - X_0 Y_0 Z_0$ as a result of the following operation $(O_n X_n Y_n Z_n) = \hat{P}_n \hat{P}_{n-1} \dots \hat{P}_1 (O_0 X_0 Y_0 Z_0)$ In Euclidean space, the matrix operations $\hat{K} = \hat{P}_n \hat{P}_{n-1} \dots \hat{P}_1$ can always be written in the following form:

$$\hat{K} = \hat{T}_{a\gamma}\hat{C}_{\gamma} \qquad \text{even } N \\ \hat{K} = \hat{T}_{r}\hat{P}_{A}\hat{C}_{r_{A}} \qquad \text{odd } N \qquad \qquad \hat{T}_{a\gamma}\hat{C}_{r}\bar{E} = \bar{E} \qquad \text{even } N \\ \hat{T}_{r}\hat{H}_{A}\hat{C}_{r_{A}}\bar{E} = \bar{E} \qquad \text{odd } N$$

$$(1)$$

Where ${}^{\Lambda}, C_{\gamma}$ indicates the operator representing rotation through an angle γ ; $\hat{T}_{a\gamma}$ represents the operator representing translation by a vector $a\gamma$; P_A indicates the operator of specular reflection in a plane M_A ; C_{rA} is the operator representing rotation through an angle γ_A , where $\gamma_A \perp M_A$; \hat{T}_r is the operator of translation by a

vector $r \in M_A$. Such an optical axis of the resonator satisfies the above-described. It is conceivable that the direction of self-conjugate ray axis coincides with the eigenvector of operation

matrices ${}^{n}, K = {}^{n}, P_{n}, P_{n-1}, ..., P_{1}$ with eigenvalue 1. But due to the changes of the terminal point of incident light on the spherical mirror will change the normal direction of spherical mirror, which will generates new rotation transformations and translation transformations. The characteristics of the conjugate axis of multi-mirrors resonator system including a spherical mirror is analyzed in detail as follows.

2.2 Misalignment sensitivity of resonators with a spherical mirror

In order to analyze the self-conjugate axis sensitivity characteristics of a multi-mirrors cavity including spherical mirrors, it is necessary to build a proper coordinate system and choose an appropriate analytical method to determine the existence of cavity self-conjugate axis and its behavior when the mirror appears angular misalignment. In this paper, a right hand coordinate system is established as shown in Figure 2.



Figure 2(a): Right-handed coordinate system O_0 - X_0 Y_0Z_0 in which the O_0 - Z_0 axis coincides with a self-conjugate ray and the O_0X_0 axis lies in the plane of incidence of the ray and its image in the resonator mirrors is the system O_n - X_n Y_nZ_n . As shown in Figure 2(a), the mirror in the system is the case of all plane mirrors, At this time, when the system has a misalignment mirror, because the normal direction of other mirrors remain unchanged , and the transformation matrix of the other mirror remains unchanged, however, when the mirrors

170

of the system contains a spherical mirror, as shown in Figure 2(b), due to the deflection of the plane mirror, the normal direction of the spherical mirror is changed, the transformation matrix of the mirror is changed too.

We suppose that mirror M_N rotates around O_0 - Y_0 through angle φ , perpendicular to the plane of incidence, corresponding, rotates the O_n - $X_nY_nZ_n$ system about the same axis through an angle 2φ , then the new image of the O_0 - $X_0Y_0Z_0$ system is denoted by O'_n - $X'_nY'_nZ'_n$, in Figure 2a, we get

$$\begin{pmatrix} \cos 2\varphi & 0 & \sin 2\varphi \\ 0 & 1 & 0 \\ -\sin 2\varphi & 0 & \cos 2\varphi \end{pmatrix} \begin{pmatrix} \cos \gamma & -\sin \gamma & 0 \\ \sin \gamma & \cos \gamma & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$
(2)

While the situation as shown in Figure 2(b), Based on Eq. (2), the transformation relationship change in the proper order, first the position of the ray changes along the incident mirror M_R rotates around the O_0 - Z_0 axis though the angle γ_R =- $L\gamma/R$, and then rotates around the O_0 - Y_0 axis though the angle φ_R =- $L2\varphi/R$, and the equation of final transformation relationship below for more details,

$$\begin{pmatrix} \cos 2\varphi_{R} & 0 & \sin 2\varphi_{R} \\ 0 & 1 & 0 \\ -\sin 2\varphi_{R} & 0 & \cos 2\varphi_{R} \end{pmatrix} \begin{pmatrix} \cos 2\varphi & 0 & \sin 2\varphi \\ 0 & 1 & 0 \\ -\sin 2\varphi & 0 & \cos 2\varphi \end{pmatrix} \begin{pmatrix} \cos \gamma & -\sin \gamma & 0 \\ \sin \gamma & \cos \gamma & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos \gamma_{R} & -\sin \gamma_{R} & 0 \\ \sin \gamma_{R} & \cos \gamma_{R} & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} a_{11}' & a_{12}' & a_{13}' \\ a_{21}' & a_{22}' & a_{23}' \\ a_{31}' & a_{32}' & a_{33}' \end{pmatrix}$$
(3)

Where φ_z and γ_z represent the total variation of the angle in the two directions of the system respectively, expressed as $\varphi_z = \varphi + \varphi_R$, $\gamma_z = \gamma + \gamma_R$. As the O₀-Z₀ axis direction is the direction of incident light, the following two equations can be obtained:

$$\begin{cases} 1 - \cos 2\varphi_z \cos \gamma_z x + \cos 2\varphi_z \sin \gamma_z y - \sin 2\varphi_z z = 0\\ -\sin \gamma_z x + (1 - \cos \gamma_z) y = 0 \end{cases}$$
(4)

The closed optical axis direction coincides with the eigenvector of the transformation matrix with eigenvalue 1, and the new closed optical axis direction can be obtained by solving the new transformation equation (3). We find the angle between the O_0 - Z_0 axis and the direction of the new closed optical axis, then the angle of the new axis α_z can be obtained as $\cos \alpha_z = \cos \varphi_z (1+\sin^2 \varphi_z \cos^2 \gamma_z/2)^{-1/2}$. It follows that the angular displacement of the self-conjugate ray depends on the rotation of the mirrors and their initial positions. The sensitivity of the resonator to the angular misalignment of the mirrors is given by $S=(d\alpha_z/d\varphi_z) | \varphi_z=0(\sin(r_z/2))^{-1}$. The above equation represents the misalignment sensitivity of cavity resonator and the self-conjugate axis deviation rate. Obviously, the above equation is expressed as the sensitivity of the vertical to the incident surface. Similarly, it can be extended to system including any numbers of spherical mirrors, then the relationship of the angle between the angles in the equation as shown below, it should be noted that the O_0 - Z_0 axis is along the direction of the self-conjugate axis, and the O_0 - Z_0 axis is rotated γ around the O_0 - Z_0 axis, and $v=\varphi$ or $v=\gamma$:

$$v_{R_i} = -\frac{L2\nu}{R_i}, \quad v_{R1} = -\frac{L2\nu}{R_i}; \quad v_{R2} = -\frac{L2\nu_1}{R_2}; \dots, \quad v_z = \nu + \sum_{i=1}^M \nu_{R_i}$$
(5)

In order to make analysis more easily, we take concrete analysis on the sensitivity expression of the resonator with only one spherical mirror, showed as :

$$S_{R} = \frac{d\alpha_{z}}{d\varphi_{z}}\Big|_{\varphi_{z}=0} = \left(\sin\frac{\gamma_{z}}{2}\right)^{-1} = \left[\sin\frac{\gamma}{2}\left(1-\frac{L}{R}\right)\right]^{-1}$$

We find that the stability condition is |1-L/R<1| when the cavity contains only one spherical mirror. It suggests that the misalignment sensitivity of resonator is increased, as well as the deviation speed of optical axis due to the spherical mirror existing. Similarly, the sensitivity is defined on the incident plane can be acquired. As only spherical mirror deflection occurs in the system, and when the condition $\gamma_z=0$ is satisfied, the cavity are very sensitive to the mirror positions at this situation, Combined with the stability of the resonant cavity, the structure parameters of the resonator can be determined easily.1) For an even number of mirrors, there is always a closed optical axis. 2) For a resonant cavity composed of an odd number of mirrors, it can be judged that there is still a probability for the existence of a closed optical axis, when the condition $\gamma_z=0$ is satisfied with a spherical mirror in the system. Next, the characteristic of the closed optical axis of a Non-planar ring resonators (NPRO) will be analyzed.

3. Modeling and analysis of closed optical axis of triangular resonator with spherical mirror

3.1. The characteristics of the self-conjugate optical axis of the accurate calibrated resonator

As shown in Figure 3(a), the appropriate coordinate system is established. Let us consider Figure 3(b) which indicates a right-handed coordinate system O-XYZ, the point O lies on the O_2 , direction of O-Z along to the line O_1O_2 . Then the O-XY lies in the plane which perpendicular to the O_1O_2 , as Figure 3(c) shown that the schematic diagram of overlooking of Figure 3(b), so there are the following expressions.



Figure 3(a): Geometrical construction of a four-sided non-planar ring resonator (NPRO) in brief ; Figure 3(b): Geometrical construction of a four-equal-sided non-planar ring resonator (NPRO), M_j (j = 1,2,3,4):reflecting mirror, $P_j(j = 1,2,3,4)$: terminal points of the resonator. β : folding angle, M_2 : spherical mirror with radius of R, M_1 , M_3 and M_4 : planar mirrors, O_1 , O_2 : the midpoints of straight lines P_1P_2 , P_2P_3 , P_3P_4 , P_4P_1 , P_1P_3 and P_2P_4 separately; the blue line represents the coordinate system; Figure 3(c): schematic diagram of overlooking, which is more convenient to understand the establishment of coordinate system; R is the radius of the spherical mirror and R_0 is the locatiocn of the sphere center. In the optical path, Each of the segments has a free-space propagation L_j (j = 1, 2, 3, 4), the total length of the cavity is L, $L=L_1+L_2+L_3+L_4$, the order of the propagation direction of the closed optical path along $L_1-L_2-L_3-L_4-L_1$, $P_j(j = 1,2,3,4)$ represents terminal points of closed light path in the resonator, and there are N1=(1,0,0),N2=(0,1,0),N3=(-1,0,0),N4=(0,-1,0).

Different from previous literatures, in this paper, we use the optical path turning reflection matrix, as follows. Considering a single general reflection with local axes at each mirror, a unit vector A_r represents the direction of incident light, and a unit vector A_f represents the direction of the reflective light. Due to mirror reflecting, the relationship between reflective light A_f and incident light A_r should meet: $A_r=E_N A_r$, where E_N is the reflection matrix: $H_N=1-2NN^T$, N is the normal unit vector of the plane mirror. It should be considered from the direction of the incident light along to the direction of the closed optical axis of the resonator in the instance of this paper. The incident light is expressed in the coordinate system of the first incident mirror M_1 , $A1=(cos\lambda sin\omega, sin\lambda sin\omega, cos\omega)^T$, where λ and ω is angle of incidence projection on the XOY, and ω is the angle between the light and the O-Z axis. According to the law of the generalized ray matrix for mirror reflection as described above, such light propagation in the four mirrors in cycle, the total change regulation can be written as:

$$A_{N} = (I - 2N_{1}N_{1}^{T})(I - 2N_{4}N_{4}^{T})(I - 2N_{3}N_{3}^{T})(I - 2N_{2}N_{2}^{T})A_{1} = \hat{E}_{N}A_{1}$$
(6)

Brought A_1 , N_1 , N_2 , N_3 into the above formula $A_N = (A_{N1}, A_{N2}, A_{N3})$, When there is a closed optical axis in the resonator cavity, it is required to meet $A_N = A_1$. The total round- reflection-trip matrix of a ring resonator is the linkage of each individual mirror reflection matrix in proper sequential order, and E_N represents the operator of total round-reflection-trip. Once the relationship between the optical axis direction and the round-trip matrix is established, one may find the direction of self-conjugate axis coincides with the eigenvector of the operator E_N with eigenvalue 1,

3.2. Mirror Misalignment

A The incident plane mirror P1 misalignment

As shown in Figure.4, the tilted angular misalignment causes a rotation of the optical axis from solid line to short dashed, and set the angle between the new axis and original axis to be $\Delta\lambda$ on the XOY. Let us consider the case that the incident plane mirror P1 rotates through a certain angle $\Delta\beta$ about the *O*-*Y* axis. In our setting, clockwise rotation is positive directions, it should be noted that the changes in the normal direction of spherical mirror is not only related to the deflection of a plane mirror, but also depends on the new direction of closed-optical-axis in the system. In order to express easily, we assume that all of the mirrors lie on the same plane, in the coordinate system established above, the normal vector of the offset mirror M₁ is expressed as :

	$\cos \Delta \varphi$	$-\sin\Delta\varphi$	0)	$\cos \Delta \beta$	0	$\sin \Delta \beta$		
N1s'=	$\sin\Delta\varphi$	$\cos\Delta\varphi$	0	0	1	0	11	(
	0	0	1)	$-\sin \Delta \beta$	0	$\cos \Delta \beta$		

The matrix form of this operator is $\hat{E}'_{N1} = (1-2N'_{1s}N'^{T}_{1s})(1-2N_{4s}N^{T}_{4s})(1-2N_{3s}N^{T}_{3s})(1-2N_{2s}N^{T}_{2s})$, the total round-trip matrix of a resonator can be applied used in the following areas.



Figure 4(a): Schematic diagram of experimental result on optical-axis perturbation caused by plane mirror's displacements in NPRO; the blue line represents the misalignment situation Figure 4(b) schematic diagram of experimental result on optical-axis perturbation caused by only spherical mirror's displacements in NPRO, Clearly, be similar with 4(a).

The unit vector in the direction of the closed optical axis is $A_R = (\cos\lambda \sin\omega, \sin\lambda \sin\omega, \cos\omega)^T$ so there is $A_{NR} = \hat{E}_N A_R$, where λ is angle of incidence projection on the XOY, and ω is the angle between the light and the O-Z axis, set $A_{NR} = [A_{NR1}, A_{NR2}, A_{NR3}]^T = \hat{E}_N A_R$, we can get:

$$A_{\rm NR} = \begin{bmatrix} \cos\lambda\cos\omega(2\cos^2\Delta\beta\cos^2\Delta\varphi - 1) + \sin2\Delta\beta\cos\Delta\varphi\sin\omega - \sin2\Delta\varphi\cos^2\Delta\beta\cos\alpha\sin\lambda \\ \sin2\Delta\varphi\cos^2\Delta\beta\cos\lambda\cos\omega - \cos\alpha\sin\lambda(2\cos^2\Delta\beta\sin^2\Delta\varphi - 1) + 2\cos\Delta\beta\sin\Delta\beta\sin\Delta\varphi\sin\lambda \\ \cos2\Delta\beta\sin\omega - \sin2\Delta\beta\cos\Delta\varphi\cos\lambda\cos\omega + 2\cos\Delta\beta\cos\alpha\sin\Delta\beta\sin\Delta\varphi\sin\lambda \end{bmatrix}$$
(8)

In order to calculate the simple, only the deflection in one direction is considered, we set $\omega = \pi/2$ and the direction vector of incident ray as $A_{R1} = [\cos(\lambda + \Delta \lambda), -\sin(\lambda + \Delta \lambda), 0]$, and the angle between the new axis and original axis to be $\Delta \lambda$ on the XOY, and $A_{NR1} = E_N A_{R1}$. Let $A_{N1R3} = 0$, $A_{N1R1}/A_{1R1} = A_{N1R2}/A_{1R2}$, get the relationship between $\Delta \lambda$ and $\Delta \beta$.

B. The influence of the plane mirror angular misalignment

As mentioned above, when the system contains a spherical mirror, the position of the incident point at the spherical mirror will change coinciding with the other mirrors' misalignment, then the direction of spherical mirror normal vector changes, and the transition matrix of the optical path will change. Owing to the plane mirror M1 tilted in horizontal direction, the terminal point P2 of the spherical mirror appears translation in horizontal coherent. As a result, the normal direction of the spherical mirror will appear horizontal deviation angle $\Delta\beta_R$ corresponding around the O-X axis. and then about the O-Z axis through an angle $\Delta\varphi_R$, as Figure 5 (a), combined with the optical path turning reflection matrix, it is not difficult to analyze that when the closed-optical-axis circulate in the cavity, as a result of the angle of the plane mirror deflection, the horizontal deflection angle corresponding to the spherical lens is $\Delta\beta_R$ =- $\Delta\beta L/R$, $\Delta\varphi_R$ =-(L/R) $\Delta\varphi$. In order to calculate the simple, only the deflection in one direction is considered, we set φ =0, and the direction of the incident light is

expressed as :

$$A_{N1} = \hat{E}_{N} A_{1R} = \begin{bmatrix} \sin(\lambda + \Delta\lambda) (\sin^{2}(\Delta\beta + \Delta\beta_{R}) - \sin^{2}(\Delta\beta - \Delta\beta_{R})) + \cos 2\Delta\beta \cos(\lambda + \Delta\lambda) \\ \cos 2\Delta\beta_{R} \sin(\lambda + \Delta\lambda) \\ -\sin 2\Delta\beta \cos(\lambda + \Delta\lambda) + \cos 2\Delta\beta \sin 2\Delta\beta_{R} \sin(\lambda + \Delta\lambda) \end{bmatrix}$$
(9)

 A_{1R} = [cos(λ + $\Delta\lambda$), sin(λ + $\Delta\lambda$), 0] Let L/R=1/2, As shown in the Figure 5(b) is the relationship between $\Delta\lambda$ and $\Delta\beta$. At present, we analyzed the influence of the angle of incident angle on the cavity axis, the angle error curve of the resonator mirror is given, and the accuracy requirement can be selected according to the error curve.

It is also necessary to point out that the method used in this paper is different from the traditional ABCD ray matrix of Gaussian beam reflection, which mainly studies the beam distribution for a Gaussian beam in the plane that perpendicular to the optical axis, in general the elements of the ABCD matrices are unconcerned with the self-conjugate axis, the calculation in the literatures, whether the optical axis closed should take into analysis first when study the misalignment of mirrors.



Figure 5(a): Schematic diagram of spherical mirror's behavior with plane mirror M_1 displacement $\Delta\beta$. Figure.5(b): Schematic diagram of relationship between $\Delta\lambda$ and $\Delta\beta$, and the vertical line when $\Delta\beta=0$ as a result of \hat{E}_{N} is an unit matrix with an arbitrary angle of incidence.

4. Conclusion

The development of CRDS technology is mature and the course of commercial instrument is more than 10 years. Thanks to breakthroughs in new materials, new technology and other related fields, CRDS in recent years, whether it is in the new product launch, or in the application and promotion of the momentum of development (Berden et al., 2000) (He and Orr, 2000). In this paper, by utilizing the optical path turning reflection matrix the generalized change regulation of optic axis influenced by both the radial and axial misalignment of both plane mirror and spherical mirror in a nonplanar ring resonator have been obtained. Besides, the analysis of the optical-axis misalignment transmission that in azimuth direction and pitch direction in a nonplanar ring resonator with spherical mirror have been taken, and the corresponding angle error curve. The analysis in this paper is important to the cavity design of NPRO and it could be helpful to avoid the violent movement of the optical-axis to small misalignment of the mirrors in NPRO.

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