

Correction of Wavenumbers in a FTIR Imaging Spectrometer

A. N. Morozov^a, S. I. Svetlichnyi^b, and I. L. Fufurin^a

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Abstract—An optical scheme of an FTIR imaging spectrometer designed based on the Mickelson interferometer with a mobile mirror and multielement photodetector is constructed. A correction procedure of wavenumbers making it possible to avoid errors in the results of spectral analysis and identification of substances, as well as to attain the maximally attainable spectral resolution, which is determined only by the angular field corresponding to the size of one photodetector pixel, is proposed.

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Fourier spectrometers [1] have found numerous applications both in laboratory spectral investigations and in spectral analysis outside the laboratory. Fourier-transform IR spectrometers (FTIR spectrometers), which register the intrinsic thermal radiation of an object under study, are passive-type spectral devices and are usually used for spectral analysis outside the laboratory [2]. FTIR spectrometers possess the largest luminosity amongst all spectral devices [1] and make it possible to record the mid-resolution IR spectra for time on the order of 1 s, which gives the opportunity to form real-time remote sensing systems based on such devices [3].

In this study, we consider an FTIR imaging spectrometer [4], which is the development of a strip of FTIR spectrometers with a cooled single-element photodetector [3, 5, 6]. The FTIR imaging spectrometer allows us to acquire the distribution pattern of the substance cloud in the instantaneous field of view of a device, the width of which over the azimuth is 14° [7]. Simultaneously using two FTIR imaging spectrometers makes it possible to determine the distance to the cloud of the substance under study and its sizes [8].

One primary condition for the possibility of performing spectral analysis and identifying substances is correct labeling of the wavenumbers in reconstructed spectra, which is especially typical to analyze the spectra of low-molecular compounds (ammonia, meth-

ane, etc.) possessing narrow characteristic spectral lines. Classical FTIR spectrometers based on the Michelson interferometer have a reference laser channel in their design, which makes it possible to determine the shift of a mobile interferometer mirror with high accuracy and calculate the wavenumbers. The optical path difference of marginal interferometer rays in FTIR imaging spectrometers [7] substantially depends on the phase incursion, which is determined by the geometry of the optical system and the sizes of the multielement photodetector.

Figure 1 shows the reference spectrum of ammonia vapors (a low-molecular volatile compound having narrow spectral lines) and the spectrum recorded using a side photodetector pixel of the FTIR imaging spectrometer in the range of $1100\text{--}1170\text{ cm}^{-1}$ with a resolution of 4 cm^{-1} .

It is seen from Fig. 1 that the experimental spectrum of ammonia vapors is shifted relative to the reference one into the region of lower wavenumbers by more than 2 cm^{-1} . The correlation coefficient of the reduced spectra in the range of $700\text{--}1400\text{ cm}^{-1}$ equals 0.48, which is a very low value to identify a substance by its infrared spectrum. In order to perform the spectral analysis of low-molecular substances possessing narrow spectral lines or bands, the phase incursion in the optical path difference for the marginal interferometer rays should be taken into account and the wavenumber scale correction procedure should be performed for the reconstructed spectra.

Taking into account the phase incursion in the optical path difference for the rays that deviated from the interferometer optical axis leads to limitation of the maximally attainable spectral resolution depending on the angular sizes of the photodetector [3].

^a Moscow State Technical University named after Bauman, Vtoraya Baumanskaya ul. 5, Moscow, 107005 Russia

^b Institute of Energy Problems of Chemical Physics named after Talroze (Branch), Russian Academy of Sciences, Chernogolovka, p/o box 56, Moscow oblast, 142432 Russia
e-mail: igfil@mail.ru

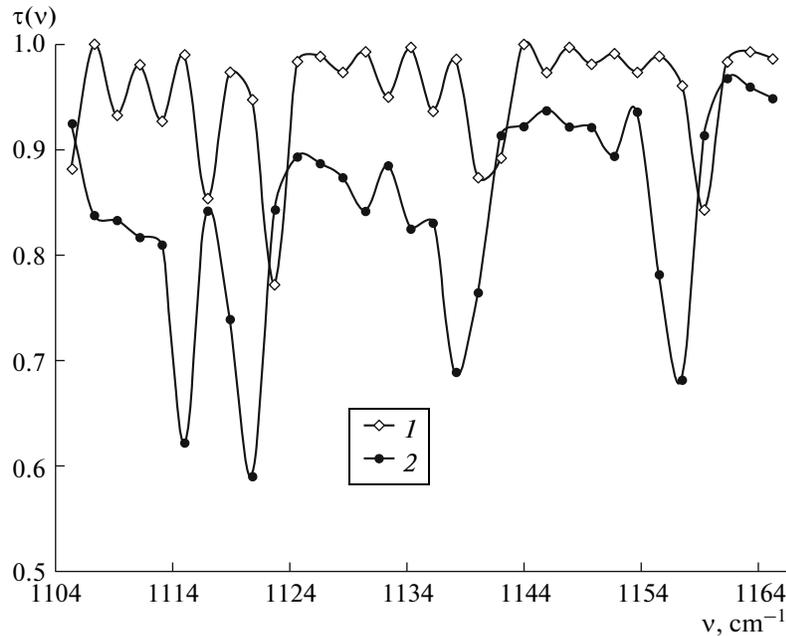


Fig. 1. (1) Reference spectrum of ammonia vapors and (2) spectrum of ammonia vapors registered by one of the side photodetector pixels.

Let us consider the nature of the phase incursion in the optical path difference for marginal interferometer rays. The design of the FTIR imaging spectrometer is based on the classical Michelson interferometer with a mobile mirror [1, 3]. Autocorrelogram $I(x)$ is fixed at each element of the multielement photodetector of the FTIR spectrometer after the modulation of the input radiation flux, based on which, the energy spectrum of input radiation $B(\nu)$ is reconstructed with the help of the inverse Fourier transform [9]:

$$B(\nu) = \int_{-\infty}^{+\infty} I(x) \cos(2\pi\nu x) dx, \quad (1)$$

where x is the path difference of the rays in an interferometer.

Figure 2 shows the passage of the marginal ray in the Michelson interferometer corresponding to the zero path difference, as well as the marginal beam path upon shifting the mobile mirror by magnitude l .

For the principal ray in the interferometer (see Fig. 2) the path difference is defined as $x = 2l$, where l is the shift of a mobile mirror from the equilibrium position corresponding to the zero path difference of rays in the interferometer.

Based on the optical layout of marginal rays in the interferometer, let us determine the optical path difference x' of marginal rays deviating by angle β from the interferometer optical axis. It follows from Fig. 2

that the optical path difference passed by marginal rays 1 and 2 will be written in the form

$$x' = \frac{2l}{\cos\beta} - 2l \tan\beta \sin\beta = 2l \cos\beta. \quad (2)$$

Then the optical path difference of the marginal and principal rays in the interferometer is associated as follows:

$$x' = x \cos\beta, \quad (3)$$

where x' is the path difference of marginal rays deviated by angle β from the interferometer optical axis and x is the path difference of principal interferometer rays.

Using the Fourier transform (1) and the relationship for the optical path difference in interferometer (3), we can write the dependence of energy spectrum $B(\nu)$ and interferogram $I(x)$ recorded in the photodetector pixel visible at angle β (see Fig. 2):

$$B(\nu) = \int_{-\infty}^{+\infty} I(x) \cos(2\pi\nu \cos\beta x) dx. \quad (4)$$

Introducing the substitution

$$\nu' = \nu \cos\beta,$$

we can write expression (1) in the form

$$B(\nu') = \int_{-\infty}^{+\infty} I(x) \cos(2\pi\nu' x) dx. \quad (5)$$

Thus, spectral lines ν' of reconstructed spectrum $B(\nu')$ for marginal rays turn out to be shifted to the

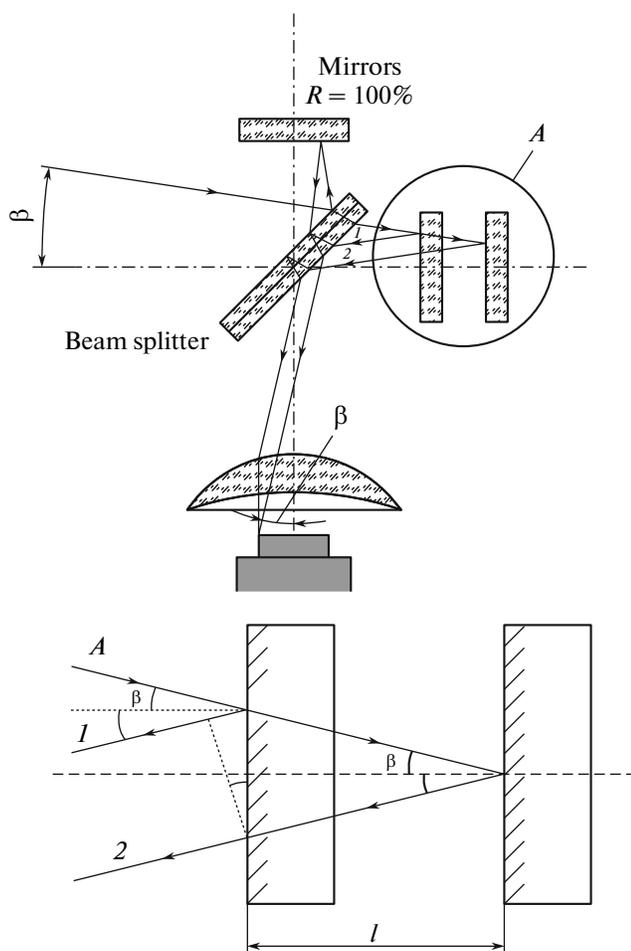


Fig. 2. Geometric marginal ray path in the interferometer (1) for the mobile mirror position corresponding to the zero optical path difference and (2) with the mirror shift by distance l .

region of lower wavenumbers relative to the initial scale of wavenumbers ν (see Fig. 1). To label wavenumbers correctly, a scale multiplier should be introduced:

$$\nu = \frac{\nu'}{\cos \beta}. \quad (6)$$

Let us consider the FTIR spectrometer [7] with a multielement cryostatted mercury cadmium telluride photodetector used in its design, the geometry of which is shown in Fig 3.

The focal distance of the photodetector collecting optics $f = 18.5$ mm. For the mentioned geometry of the photodetector and collecting optics, the shift of wavenumbers along axis $\nu' - \nu$ for side pixels is about 2 cm^{-1} in the working spectral range of $700\text{--}1400 \text{ cm}^{-1}$. The FTIR spectrometers with a cooled photodetector [6, 7] and FTIR imaging spectrometers process the infrared spectra with a resolution of 4 cm^{-1} . According to the Kotel'nikov theorem [10], discrete counts in the

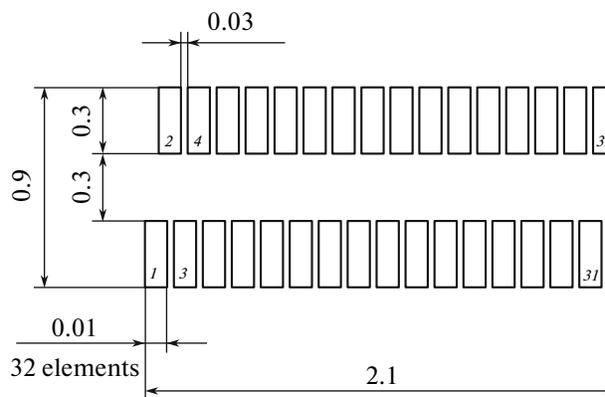


Fig. 3. Multielement photodetector design. The sizes are given in mm, and photodetector pixels are numbered from 1 to 32.

spectrum are labeled with a doubled frequency; therefore, the wavenumber shift along the axis of 2 cm^{-1} is essential to perform the spectral analysis and identify the substances (see Fig. 1).

To identify the substances by infrared mid-resolution spectra in spectral analysis problems outside the laboratory, as a rule, the correlation coefficient is used as the static correspondence parameter of the reference and registered spectra [11–13]. If the correlation coefficient exceeds the established threshold value, the substance is considered identified in this experiment. Figure 4 shows the dependence of correlation coefficient r of the reference and registered spectrum of ammonia depending on photodetector pixel number N . The correlation was calculated both for the experimental spectra without the correction and for the spectra restored allowing for the scale multiplier (6). Based on the photodetector design symmetry (Fig. 3), the dependence is presented only for the lower series of pixels.

It is seen from Fig. 4 that the correlation magnitude of the spectra registered for central and side photodetector pixels can differ twofold if no wavenumber correction procedure is performed, which critically affects the substance identification by the infrared spectrum. Moreover, it should be noted that the correlation coefficient for pixel numbers of 1, 3, and 31 is below the detection threshold, which evidences the impossibility to identify ammonium at the photodetector pixels mentioned. The performance of wavenumber correction allowing for scale multiplier (6) makes it possible to eliminate almost completely the problem of spectrum shift by wavenumbers.

In conclusion, we should note that the proposed wavenumber correction while processing the experimental data acquired using FTIR imaging spectrometers allows us to avoid errors in the results of spectral

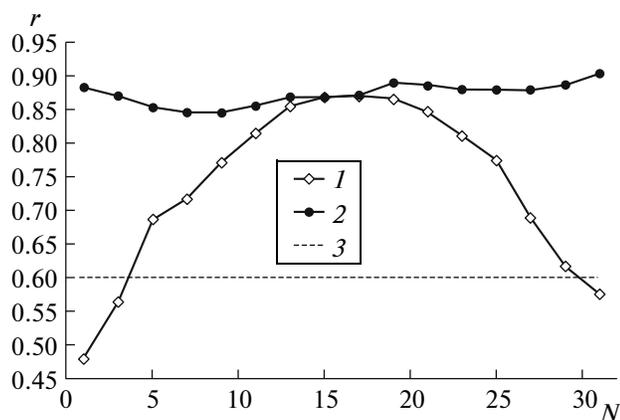


Fig. 4. Dependence of correlation r of the reference and experimental spectra of ammonia vapors (1) without the wavenumber correction procedure and (2) with the wavenumber correction. Curve (3) corresponds to the detection threshold. N is the photodetector pixel number.

analysis and identification of substances. Moreover, the performance of correction procedures allows us to gain the maximally attainable spectral resolution, which is determined only by the angular field corresponding to the size of one photodetector pixel.

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