Planar Diode Multiplier Chains for THz Spectroscopy

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Abstract—Broadband frequency multiplier chains based on planar GaAs Schottky diodes [1], developed for the Herschel Space Observatory (Herschel) [2] and ALMA [3], have been applied to high-resolution laboratory spectroscopy covering most frequencies from 0.2 to 2.5 THz. These chains are driven by commercially available frequency synthesizers and millimeter wave multipliers (6x), which provided a broadband RF source with several mW from 70 to 120 GHz. The millimeter wave signal is amplified with recently developed power amplifiers [4] to more than 100 mW with 15% bandwidth to drive cascaded multipliers [5]–[8]. These multipliers are cascaded with up to 4 successive doublers and triplers with a multiplication factor of 2 to 36. By selecting well-matched multiplication stages, sufficient power over a 10% bandwidth is generated.

High-resolution laboratory spectroscopy is utilized as a diagnostic tool to determine noise and harmonic content of balanced [9]–[11] and unbalanced [12]–[14] multiplier designs. Balanced multiplier designs suppress unintended harmonics more than -20 dB. Much smaller values were measured on unbalanced multipliers.

Index Terms—high-resolution spectroscopy, THz, cascaded frequency multipliers, planar GaAs Schottky diode, noise level and harmonic content

I. INTRODUCTION

The development of all-solid-state frequency sources for HIFI (Heterodyne Instrument for the Far-Infrared) and ALMA (Atacama Large Millimeter Array) has provided broadband RF sources without mechanical tuners in the THz regime. Frequency coverage is central in all remote sensing experiments. Historically atmospheric chemistry instruments like MLS [15] have relied on wide band IF mixers to achieve coverage while astrophysics missions like SOFIA [16] and ALMA [3], and Herschel use both wide band mixers and multiple local oscillator sources. In all cases, precise frequency knowledge and spectral purity must be maintained in order to make accurate observations of molecular and atomic transitions. Laboratory high-resolution spectroscopy provides atomic and molecular data that enables interpretation of atmospheric chemistry observations, remote and local planetary observations, and spectroscopic astrophysical observations.

The challenges in laboratory spectroscopy are similar to the remote sensing one in terms of the need for bandwidth and spectral purity, but there is a difference in that the spectrometer can be re-adjusted by the operator as needed. Unfortunately such re-adjustment is time-consuming and effectively prevents collection of comprehensive self-consistent data sets. A primary limitation in traditional millimeter and submillimeter spectrometers is the tuning range of the phase lock loop. In this case a commercially available frequency synthesizer with its high quality internal lock loop was utilized. If the spectral purity of the synthesizer is sufficient, direct multiplication with planar multipliers and MMIC amplifiers, described herein, allows nearly autonomous operation for rapid collection of data at sub-millimeter wavelengths [18]. As a demonstration, we conducted a series of high-resolution spectra of rotational transitions of isotomers of H$_2$O (water), HOC$_1$(hypochlorous acid), and CH$_3$OH (methanol).

In addition, the spectroscopic techniques provide information on the harmonic content and the noise level of the signal source. In local oscillator applications, it is very important to suppress the harmonic content, especially the higher frequency ones which cannot be cut-off by the output waveguide. Balanced multiplier, which can be designed in a symmetric or anti-symmetric configuration, allow to reduce the higher harmonics per design. In these designs the symmetry prevents unwanted odd or even harmonics to the order of -20 dB to -30 dB. It has been observed that the bias conditions impact the harmonic generation strongly in all tested multipliers. This is especially true in unbalanced designs where unwanted harmonics could be higher than the designed ones. However, designs with balanced diode configurations have demonstrated good suppression of unwanted harmonics even when operated at bias conditions which were not the nominal ones. This is very important when high spectral purity of the LO [19] is required, as it is the case for laboratory spectroscopy and in heterodyne systems using wideband Hot Electron Bolometers (HEB). An additional consideration in both applications as laboratory and remote sensing is that a HEB is sensitive to amplitude modulation (AM) of incident RF power. AM noise at the modulation frequency impacts the signal to noise ratio in direct detecting systems as well as in
heterodyne systems. Additionally, in heterodyne systems the system stability is reduced by AM noise because the receiver gain is modulated which prevents efficient integration of the signal. Higher harmonics are spurious signals [20], which can introduce ghost-lines making interpretation of the data more difficult or impossible. In order to characterize the local oscillators two different spectrometers, described in the next sections, were utilized.

II. SPECTROMETER

A. General Description

One of the important components in a spectrometer or a receiver system is a frequency locked source with knowledge of the precise frequency (figure 1).

A frequency standard with an accuracy of at least a factor 10x higher than the targeted resolution of the spectrometer is required. In the laboratory this translates to at least a part in 10^{9} while some wide line remote sensing applications only require a part in 10^{6}. Further, the close-in spectral purity of the reference source is multiplied to higher harmonics and impacts the noise floor when the reference has high noise levels. When using a highly pure fundamental oscillator, at higher frequency the requirements on the noise in the lock loop of a multiplier chain can be minimized. This approach is used in the Cologne spectrometer. In the JPL spectrometer a fundamental oscillator at X-band frequencies is used, while most radio observatories lock the local oscillator with millimeter wave Gunn oscillators. Since amplification and multiplication can degrade spectral purity and introduce spurs, the fundamental oscillator ultimately limits the spectral purity that the spectrometer or local oscillator can achieve.

In the laboratory the generated RF signal propagates through a gas cell before the signal reaches a sensitive detector. A variety of modulation techniques, AM, FM, and combinations thereof, can be combined with lock-in amplifiers to minimize instrumental effects. Laboratory spectroscopy is generally performed in absorption, but if heterodyne detection is used it can be done in emission as well. Two different implementations of submillimeter spectrometers are described in the following sections.

B. Cologne THz spectrometer

The Cologne THz spectrometer uses a series of different backward wave oscillators (BWO) as fundamental oscillators. Since BWOs typically generate mW power levels coupled into an overmoded waveguide, they are mostly used to pump quasi-optical frequency multipliers. Figure 2 shows the Cologne spectrometer and its phase-lock loop, which uses a subharmonic mixer that mixes a multiple of a millimeter wave synthesizer signal quasi-optically with a fraction of the BWO power. The difference in frequency is amplified and fed to a PLL (Phase Lock Loop), which provides the control signal at 350 MHz to frequency-lock the BWO. Since BWOs have very high intrinsic spectral purity, the bandwidth of the lock-loop is dominated by the need to follow the modulation applied to the synthesizer. Matching optics was designed to optimize the coupling of the RF beams. The one limitation of the BWO system is the voltage compliance of the lock loop which allows for approximately 1 GHz of tuning at the output frequency before the lock loop requires re-adjustment.

The Cologne spectrometer takes advantage of the spectral purity of the BWO. This characteristic and the use of a subharmonic mixer which generates very little or no output at the BWO frequency, assure that the spectrometer system is free of spurious signals except a nearly negligible (<30dB) [21] amount of 2nd harmonic from the BWO. A disadvantage of this approach is that the spectrometer is not frequency-lock the BWO. Since BWOs have very high intrinsic spectral purity, the bandwidth of the lock-loop is dominated by the need to follow the modulation applied to the synthesizer. Matching optics was designed to optimize the coupling of the RF beams. The one limitation of the BWO system is the voltage compliance of the lock loop which allows for approximately 1 GHz of tuning at the output frequency before the lock loop requires re-adjustment.

The BWOs have been successfully used with multiplier technology in the past [13]. As a result, the first test of several multipliers developed for HIFI could be performed by using BWO's, because solid-state pump multiplier chains at frequencies from 806 to 900 GHz were still under development. The spectrometer in Cologne was utilized to characterize 1.9 THz triplers and 2.7 THz triplers. With this spectrometer, transition frequencies up to 2.3 THz were observed on different molecules.

C. JPL Frequency Multiplier Submillimeter Spectrometer

The spectrometer at JPL utilizes a fundamentally different approach from the one in Cologne. The spectrometer is built around a commercial core of microwave and millimeter components and relies on direct multiplication and amplification to the submillimeter and THz frequencies. In

Fig. 1. Block diagram of spectrometer.

Fig. 2. Block diagram of Cologne THz Multiplier spectrometer.
this approach, it is not possible to use the intrinsic spectral purity of a millimeter or submillimeter fundamental oscillator and PLL to clean-up the signal. As a result, the fundamental requirement is that the input signal is spectrally pure and as free of spurs as possible. The advantage to the approach is that the spectrometer requires only one lock loop that is under this approach, it is not possible to use the intrinsic spectral purity and PLL to clean-up the signal. The input power of the x12 multiplier was provided by a 100-250mW 71-82 GHz amplifier and the x8 by a 100-200mW 100-108 amplifier. This signal was multiplied by frequency doublers or triplers up to the THz range. Several fraction of one microwatt at THz frequencies were sufficient to perform sensitive spectroscopy. Coverage of 400-720 GHz was achieved with two Virginia Diodes multipliers. The x8 JPL chain can be used to cover 720-840 [11], a x10 VDI chain covers 770-860 GHz, the JPL x12 covers 840-960 GHz, a JPL x12 covers 1060-1220 GHz [22] and a JPL x18 covers 1575-1700 GHz [23].

IV. SPECTROSCOPY

Ultimately most submillimeter frequency multipliers are used to perform spectroscopy with a receiver. However, laboratory spectroscopic applications can provide a wealth of detailed information on the source performance. The next section discusses a number of multiplier measurements that can be achieved spectroscopically.

A. Power bandwidth

The most important characteristic of any submillimeter source is the power bandwidth, which is determined once the RF output in CW mode is maximized at nominal bias parameters. For this characterization, the bias conditions on the frequency multipliers are adjusted to be in the safe range [24] over the entire frequency scan. Safe bias conditions are defined that no excessive forward currents or any reverse currents are induced in the multiplier diodes while the frequency is incrementally changed at constant RF input level. To determine the total power content in a spectrometer setup, the RF signal is AM modulated. If the dynamic range of the detector is exceeded, the power may be attenuated. In most of the cases several sheets of paper are sufficient to prevent saturation of the detector. The total power measurement gives the shape of the

III. CASCADEd FREQUENCY CHAINS

Many of the solid-state frequency chains used in the JPL spectrometer were developed for the HIFI instrument of Herschel. Each chain contains a cascade of three or four frequency doublers or triplers starting from W-band. These modules [6] were designed for wide band operation at 120 K and high efficient power conversion without mechanical

turners. Only electrical tuning with the bias supply is required, which simplifies the operation and enables computer control. Nearly 80% of frequency coverage between 0.15 to 2 THz and partial coverage from 2.4 to 2.7 THz were achieved by cascading a x8 or x12 chain with a single diode doubler/tripler. The input power of the x12 multiplier was provided by a 100-250mW 71-82 GHz amplifier and the x8 by a 100-200mW 100-108 amplifier. This signal was multiplied by frequency doublers or triplers up to the THz range. Several fraction of one microwatt at THz frequencies were sufficient to perform sensitive spectroscopy. Coverage of 400-720 GHz was achieved with two Virginia Diodes multipliers. The x8 JPL chain can be used to cover 720-840 [11], a x10 VDI chain covers 770-860 GHz, the JPL x12 covers 840-960 GHz, a JPL x12 covers 1060-1220 GHz [22] and a JPL x18 covers 1575-1700 GHz [23].

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output power convolved with the frequency dependent throughput and the characteristic of the optics, sensitivity of the detector, and atmospheric absorption. Once care has been taken to minimize the frequency dependent effects, the multiplier pass band can be determined. For quantitative measurements the detector’s responsivity has to be known.

In Figure 4 a total power sweep of a 1600 GHz frequency chain is displayed. The measurement was performed through a 1.6 meter long gas cell with 150 mTorr of methanol. The step size was 2.5 MHz or about 20 times higher resolution than the one available for the Fourier transform infrared spectrometer system. The red stick spectra present the predicted methanol ground state lines and relative intensity. The frequency coverage can be extracted from the data once the effects of the atmosphere’s absorption are accounted for. In this case the dip in the middle is due to a strong water absorption line located at 1.604 GHz and the RF characteristic of the last stage multiplier. When the optical path is purged with dry Nitrogen, the absorption will be reduced.

**B. Extraction of noise level and harmonic content**

One important consideration for multipliers is to investigate whether the total amount of power is generated in the desired harmonic. For this matter, spectroscopy on well known molecular transitions has to be performed.

The line strength of molecular transitions can be determined with high accuracy by measuring the electric dipole moment and applying the selection rules [25] for the transition. The JPL spectral line catalog [26] and the CDMS [27] provide the line strength for many molecules in Log(I(T)) format where the temperature (T) is 300 Kelvin. The peak absorption for pressure broadened lines is

\[
\alpha_{\text{max}} = \frac{I(T)}{\Delta v} \left( \sum \frac{T_0}{T} \right) \times 102.458 \text{cm}^{-1}. \tag{1}
\]

Here \(\Delta v\) is the half width at half height of the line at 1 Torr in MHz. The peak absorption for pressure broadened lines is

\[
\alpha_{\text{max}} = 4.3429 dB. \tag{2}
\]

Since the catalogs generally do not include the contribution for excited vibrational states the line strength should be divided by the vibrational partition function given below:

\[
Q_v = \left( \sum e^{-\epsilon_i/kT} \right) \left( \sum e^{-\epsilon_{2i}/kT} \right), \tag{3}
\]

where the \(v_i\) is the number of quanta in the i-th of the 3N-6 vibrational modes. Vibrational states above 1000 cm\(^{-1}\) (wavenumber, cm\(^{-1}\) is equal to 29.97925 GHz) in energy contribute less than a 1% correction. When this is done for the Q branch feature in figure 5, the absorption is expected to be between 18.9 and 19.7 dB in the band head in good agreement with the observed transmission. A note of caution is that the detector must be sensitive to the other possible harmonics as well. This technique determines only if there is power at other frequencies, but it cannot distinguish between noise and harmonic content.

**C. Harmonic content**

The harmonic content can be directly determined by spectroscopic measurements on known molecules with relatively strong absorption features with known frequencies and intensities in all the possible harmonics. The spectrum is measured, then, at low pressure with FM or tone burst modulation. The harmonic content can be determined by the ratio of the expected line strength in the fundamental harmonic to the other harmonics.

The spectrum in Figure 6 is the one for N\(_2\)O in natural isotopic abundance in the frequency range from 1.0891 THz to 1.0907 THz. The 18-O has a 0.25% natural abundance and the 15-N isotope of one of the nitrogen atoms has an abundance of 0.36%. Considering the envelope of the total power we determined a content of 27 (±/2) dB from the fourth harmonic on a balanced 1.2 THz tripler [22]. A rich molecular spectra is required to perform a complete analysis of the pass band. This measurement is an example of how to estimate the harmonic power content.

A suppression of more than 20 dB has been measured for every tested balanced multiplier designs including doublers, triplers, and quintuplers. In these designs even or odd harmonics are suppressed internally in the circuit. This suppression is essential to reduce the contribution of the next
higher harmonic efficiently. In the unbalanced designs, such as single diode configurations, the next higher harmonic cannot be suppressed by the circuit symmetry. Just about all the multiplier designs with matching waveguide structure possess a common design feature which is the cut-off of the lower harmonics by the output waveguide, but all the higher contents can propagate to the output. The generation of harmonics is strongly frequency dependent, tunable by the bias point, and impacted by the level of input RF power.

In Figure 6 the harmonic content of a 1200 GHz chain with two doublers and one tripler is measured to be ~27 dB. In comparison to this value, the harmonic content of a single diode circuit a 2.7 THz tripler could be changed from -6dB to the next lower harmonic (second) being much stronger than the targeted third harmonic. Initially, the low expected power available at 800-900 GHz suggested that a single diode would work more efficiently than a design with several diodes. Further, the difficulty in terminating unwanted harmonics should be appropriately considered in any such trade-off. Currently, power levels on the order of 1 mW at these frequencies suggest that balanced configurations with two diodes at frequencies above 2 THz is now the better design option than the single diode configuration.

D. Noise level

One of the important considerations in designing a receiver is the expected noise level of the local oscillator. In an ideal design it should contribute negligibly to the overall receiver temperature. These receivers utilize SIS or HEB [28] mixers which are the most sensitive detectors up-to-date to test the noise of the LO. However, there are also a number of spectroscopic techniques that can be used to determine if the noise level is significant.

Any source suitable for use as a local oscillator should be noise-limited by the detector in spectrometers. In this case the signal to noise ratio of the detected spectra will improve in proportion to the Noise Equivalent Power (NEP) of the detector used. However, the contribution of the thermal background at 300 Kelvin limits the detector sensitivity. Without appropriate filters there is no benefit on NEPs better than $10^{-8}$, which is substantially worse than narrow banded heterodyne detection. A series of measurements with progressively more sensitive detectors can be made to verify that the signal to noise ratio on weak features improves as expected. The result of this method can’t prove that the source will work as a local oscillator, but is will indicate if the source has high noise content.

The other concern is the phase noise generated when frequency multipliers are cascaded. Since the observed spectra are a convolution of the line width of the signal source and the line width of the observed molecule, a quantitative measurement of the signal source line width is possible. Molecular spectra pressure broadens according to the linear relationship:

$$\Delta \nu = 1/2\pi \tau.$$  \hspace{1cm} (4)

where $\tau$ is the mean time between collisions. Since the Doppler contribution to the line width is directly calculable from the temperature at atomic weight, plotting the pressure broadened line width using AM modulation corrected for Doppler effects will give a slope and a zero intercept. The slope is the pressure broadening constant and the intercept is a measure of source line width [29]. Due to measurement uncertainties the accuracy is generally a few % of the molecular Doppler line width, but this method is sufficient to identify real problems with the phase noise.

E. Molecular Spectroscopy

An advantage of wide frequency range molecular data sets is the ability to apply infrared techniques where all the absorption or emission lines within the frequency range are measured. Once this is performed, computer aided methods can be used to determine the relationship between observed and calculated transitions. This is especially important when very complex spectra of traditional molecular models can not describe the existing quantum mechanic model of the molecule investigated. This allows for extension of existing databases to include more rotational and vibrational states at higher quantum numbers. Since most of the existing molecular constants cannot be used to extrapolate accurate transition frequencies (see figure 7) over the frequency ranges of Herschel, ALMA and SOFIA, it is necessary for exact astronomical interpretation of spectra to perform laboratory measurements in the THz regime of molecules of interest.

![Fig. 7: Comparison of predicted and measured transitions of methanol between 902.6 to 902.9 GHz. The difference in frequency is more than the linewidth of the transitions.](image)

V. CONCLUSION

The availability of all-solid-state frequency sources enables “IR” spectroscopy techniques to be used in the far-infrared frequency regime. With broadband frequency sweeps at THz frequencies, molecular and atomic transitions can be detected efficiently allowing computer aided processing and identification of more states and energy levels. The outcome is that precise predictions above 2 THz will be achieved, which are essential for interpretation of all radio astronomy data and the planning of future missions like SAFIR [30]. Further, spectroscopy provides a powerful diagnostic tool for characterization of the bandwidth, spectral purity, noise level, and the harmonic content of local oscillator sources. The characterization of a number of LO chains for the HIFI instrument demonstrated that balanced multiplier designs have
surprisingly sufficient suppression of higher harmonics for example 2nd, 3rd, 4th etc., while those with unbalanced designs can be remarkable poor. A conclusion of this study is that extreme care should be taken to limit the harmonics content of local oscillators in HEB applications, where ghosts lines could be observed with harmonic content which are more than 60 dB below the carrier. This will be a great challenge for any multiplier to overcome and should be considered in the design of the receiver system.

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