

ULTRASENSITIVE WIDEBAND INTEGRATED SPECTROMETER FOR CHEMICAL AND BIOLOGICAL AGENT DETECTION

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A novel concept of a compact mm/submm integrated spectrometers for environmental monitoring for hazardous materials of chemical and biological origin as well as for remote monitoring of the Earth atmosphere is discussed. The agents will be exactly identified by their unique spectral signatures. The assembled on a multi-chip module, cryocooler-mounted Superconducting Integrated SPectrometer (SISP) exploits the superior performance of superconducting Josephson junction technology and unique on-chip integration of analog components, analog-to-digital converter, and digital components. Analog components include a superconductor-insulator-superconductor (SIS) mixer with integrated quasioptical antenna, mm-wave local oscillator, and SQUID amplifier for the down-converted (IF) signals. Upon amplification, the IF signal is digitized using a bandpass delta-sigma modulator, followed by real time processing with rapid single flux quantum (RSFQ) circuitry. Experimental results showing both operation of spectrometer components and the way to their successful integration are presented.

Keywords: Biological and chemical agents, remote detection, sensing and imaging, millimeter and submillimeter wave, THz spectrometer, superconductor, RSFQ.

1. Introduction

Lightweight and compact ultra-sensitive submm integrated spectrometer is very attractive for environmental monitoring for hazardous materials of chemical and biological origin, radio-astronomical research and remote monitoring of the Earth atmosphere. The Superconducting Integrated SPectrometer (SISP) offers a unique on-chip integration of different planar components such as a SIS (superconductor-insulator-superconductor) mixer with quasioptical antenna, a superconducting local oscillator (LO), an intermediate frequency (IF) SQUID amplifier and the circuits for digitizing of down converted signals and their real time processing.

Over the past years, the proliferation of chemical and biological agents as instruments of warfare and terrorism has become a major national security issue. The threat of chemical/biological terrorist attack after the September 11th 2001 and the 1995 nerve gas attack in Tokyo underscore the need for reliable instruments capable of detecting dangerous or potentially lethal chemical and biological agents. The new ambitious radio-astronomy multi-dish projects would gain considerably by using a single-chip SISP due

to their low price and better serviceability as compared to conventional approaches. Finally, a remote study of atmospheric pollution is possible by using air or satellite borne SISP in order to detect the spectrum lines of elements.

A lot of activities recently arise in both the technology and scientific arenas associated with the THz frequencies—i.e., usually defined as the portion of the submillimeter-wavelength electromagnetic spectrum between approximately 1 mm (300 GHz) and 100 μm (3 THz). The THz regime inherently offers important technical advantages such as component compactness, wider bandwidths and improved spatial resolutions when compared to RF electronics and holds the promise for new and novel sensing applications (e.g., chemical and biological agent detection, inspection of sealed packages, concealed weapons detection, medical diagnostics, etc.). However, the same THz regime presents significant challenges such as extreme atmospheric attenuation, weak interaction signatures and standing wave interference to name a few for practical implementation within traditional scenarios. There are also scientific and engineering problems that have to date either prohibited or severely limited the implementation of conventional electronics within this regime where wavelength is on the order of component size. In addition, there are the strong scientific payoffs of the THz regime, which is the most richly populated portion of the spectrum in terms of spectral signature information. As an example, interstellar dust (which contains an array of light to heavy molecules) was predicted long ago to contain literally tens of thousands of individual spectral lines. However, only a few thousands have been resolved and many have not yet even been identified¹.

In this paper, we propose to use the same proven spectroscopic approach further advanced by unsurpassed speed of superconductor digital electronics for the real-time DSP for identification of chemical and biological agents. These same spectral signatures, which are so interesting for interstellar and intragalactic science, are also present in planetary atmospheres and therefore have relevance for atmospheric monitoring applications. The unique physical properties associated with how THz radiation interacts with matter (i.e., molecular resonances) have fueled a long term focus on laboratory-based molecular spectral analysis and on astronomical and atmospheric remote sensing.

The SIS mixer itself is undoubtedly the device of choice for a low noise front-end detector at THz frequencies. Since the noise temperature of an SIS mixer is ultimately limited only by the fundamental quantum value hf/k^2 , SIS heterodyne spectrometers have been successfully used in radio astronomy for observation of spectra with the lowest possible noise temperature in the mm and sub-mm wave range. Many applications lack a compact and easily tunable submm LO. At frequencies above 30 GHz there is a steep increase in the cost and complexity of solid state radiation sources. Gunn diodes are widely used as LOs. They have highest fundamental frequency of operation between commercially available mm wave sources up to 110 GHz. Extension to higher frequencies requires low efficiency harmonic generators. Moreover, Gunn diode sources are voltage tunable over a range typically less than $\pm 10\%$ of the resonant frequency of the oscillator. This tuning range is inadequate for many applications. We propose to use unidirectional fluxon (flux quantum $\Phi_0=h/2e$) propagation in a long Josephson tunnel junction (LJJ) as a way to achieve practical and compact on-chip LO. This is Flux-Flow Oscillators (FFOs) that satisfy the following important requirements: they deliver enough power to pump a mixer and have high frequency tunability. For standard superconducting technology when Nb is used to fabricate the FFO, such an oscillator can

be tuned from 0 to 700 GHz. For other superconducting materials (such as NbN) the upper frequency can be increased to over 1 THz. As the result of this tunability, the same integrated spectrometer can be used for chemical/biological agent detection in extremely wide (from 0 to 1THz) frequency range.

The characteristics of two *Bacillus globigii* (BG) signatures (see review by Woolard et al³) prove real viability of the proposed SISP approach. BG has signatures at ~260 GHz and ~420 GHz with signature width depending from BG form (dense, diluted and aerosol) from 6 GHz to 30 GHz³. These characteristics are very good match for proposed SISP approach. Harmless to humans, BG is ubiquitous and found easily in samplings of wind-borne dust. BG is safely used in biological studies as a stand-in for pathogenic bacteria. BG is used as a biological tracer for anthrax because its particle size and dispersal characteristics are similar to those of anthrax. A household bleach-and-water solution easily kills BG.

Digital low-temperature superconductor (LTS) technology, using rapid single flux quantum (RSFQ) logic, is the fastest integrated circuit (IC) technology today. Individual logic gates operating at 750 GHz have been demonstrated in this technology⁴. Large-scale integrated circuits with thousands of gates are being routinely manufactured at the HYPRES superconductor electronics (SCE) facility. These complex circuits exhibit synchronous operation with clock rates of 20 GHz⁵ and are expected to increase up to 40 GHz with on-going fabrication enhancements. Such performance is well beyond any other IC technology. SCE is also an extremely low-energy digital technology. Switching energy of only 10^{-18} J/gate results in negligible power dissipation (~100 nW) even at clock rates of 100 GHz. Moreover, the fundamental quantum mechanical nature of RSFQ logic ensures high-fidelity data conversion between analog and digital formats, resulting in very high linearity analog-to-digital converters.

The specific benefits of superconducting integrated spectrometer technology for chemical and biological agent detection are:

- **Precise Agent Identification** – The chemical and biological agents will be exactly identified by their unique fingerprint - their spectral signatures.
- **Enhanced Sensitivity** – The noise temperature of the wideband cryogenic spectrometer is dramatically smaller (from a factor of 4 to as much as a factor of 25 depending on the bandwidth) than a conventional spectrometer, with the advantage of being greater for wider bandwidths. This makes possible detection of lower concentration of chemical and biological agents.
- **Both Passive and Active Spectrometer** – The spectrometer may employ both the passive and active architecture. In former case it would provide spectra excited by ambient conditions (sun light, normal temperature...) and not require powerful excitation source. In later case external excitation (e.g. by GaAs Schottky diode) may be provided.
- **Ultra-wideband Agent Detection** – Use of long Josephson junctions as continually tunable LOs will allow dc-to-sub THz spectrometry.
- **Compactness** – The whole spectrometer will be implemented on a few $10 \times 10 \text{ mm}^2$ and $5 \times 5 \text{ mm}^2$ chips mounted on the multi-chip module.
- **Low Cost and High Reliability** – All components of the spectrometer are fabricated using standard low-cost, thin film, all Nb fabrication process. The final product is packaged in an ultra-reliable cryocooler with a Mean-Time-Between-Failures (MTBF) exceeding 99 years. Superconductor circuits are extremely radiation-hard, which make them attractive for space applications.

The concept of an integrated spectrometer is not new. It was first suggested by Koshelets and Shitov⁶ (see also references therein) and further developed by us⁷. The efforts in its development targeted the successful on-chip integration of such *analog* components as LO and SIS mixer with quasioptical antenna⁶. In this paper we propose a real breakthrough with the integration of superconducting thin film *analog* components (LO with phase-lock loop, mixer, and IF amplifier) with superconducting *digital* RSFQ circuitry on a multi-chip module (MCM). This spectrometer MCM will be packaged on cryocooler.

2. Integrated Digital Spectrometer

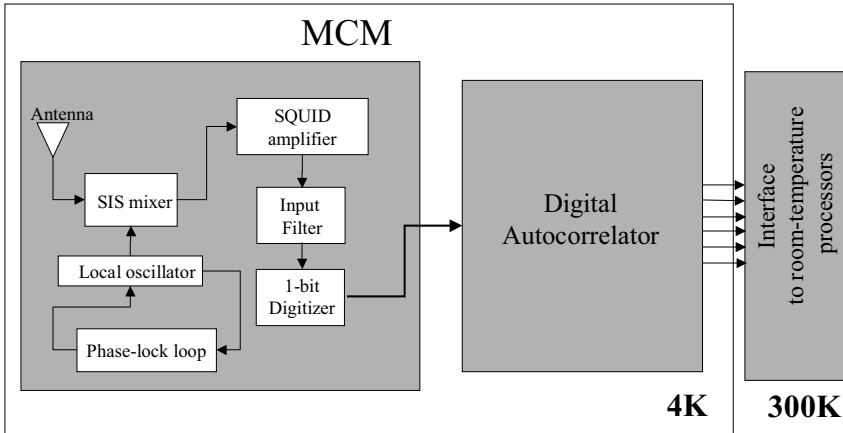


Fig. 1. The block diagram of integrated spectrometer mounted on MCM module. See text for more details.

Fig. 1 shows the block diagram of the integrated spectrometer under development. The superconducting part of the receiver consists of two chips mounted on a multi-chip module (MCM).

This chip die sizes are 5×5 and 10×10 mm². The first chip (5×5 mm²) of the spectrometer, the “front-end” chip, has the local oscillator together with the SIS mixer and impedance matching structure for better power delivery and to tune out the SIS junction capacitance. The frequency resolution of SISP determined by both the instant linewidth of the LO and its long-time stability along with the noise temperature is one of the major parameters in spectral measurements. The phase-lock loop consisted both on-chip circuitry and room-temperature electronics is employed.⁸

The first part of digital circuitry consists of a simple, fast ADC that takes the IF analog output and generates a one-bit digital pulse code at a clock rate of the order of 20 GHz or greater. The typical noise temperature of the 1-bit digitizer is of the order of few hundred K. This is significantly higher than the noise temperature of about 40 K at 475 GHz for a reference SIS mixer pumped by an external local oscillator⁶. Therefore, an IF amplifier with a power gain G_A of about 10 dB and a noise temperature T_N of about 100 K necessary to achieve the best possible overall noise temperature is designed on the same front-end chip. An IF amplifier is attached to an IF port of SIS mixer, since it helps to avoid losses of the long cable. A semiconducting IF amplifier ‘integrated’ with SIS mixer has a drawback of significant heat load (typically 20mW per stage). This makes an RF amplifier based on a SQUID that has an ultra-low power consumption, small size and

“natural” compatibility with any SIS based structure a natural choice for integration with SIS mixer.

The second chip (10 X 10 mm²) has a digital-signal processing circuit - the digital autocorrelator. We have selected the correlator circuit as the core component of our digital signal processor. One classic way to obtain the frequency spectrum of a time-domain signal $f(t)$ is to take the correlation between $f(t)$ and a time-delayed version of the same function $f(t-\tau)$. The autocorrelation function is then given by $R(\tau) = \frac{1}{T} \int f(t)f(t-\tau)dt$, where the integral is over a long time period T . That will selectively increase coherent frequency components that are periodic with time τ ; other components will exhibit a random walk. The power spectral density function $S(f)$ (or simply the spectrum of the signal) is then the Fourier transform of $R(\tau)$. If the signal is first digitized, then both the autocorrelation and the Fourier transform can be obtained in the discrete digital domain. The resolutions in the time and frequency domains are similar.

For a rapidly changing signal, this correlation function must be computed in real-time, by using a large number of correlators and accumulators in parallel. These parallel channels with distinct delays are generally known as “lags”. However, for radiometric imaging, the spectrum of the signal is relatively stable and changes only very slowly. In this case, one can compute $R(\tau)$ serially for various discrete values of τ , and then Fourier transform to obtain the spectrum. This is particularly true for RSFQ electronics, where the serial computations are so fast. This approach has the advantage of minimizing the circuit area, total power consumption, and the number of input/output (I/O) lines.

As an example, a 128-channel autocorrelator formed by 16-lag autocorrelator and a 112-bit programmable delay shift register (PRSR) was designed, fabricated and successfully tested. The PRSR acts as programmable (in increments of 16) delay line; data flow from a 16-lag autocorrelator to the PRSR and then come back.

The experimental results pertinent to front-end chip and digital autocorrelator follow in next paper sections.

3. Front-End Chip

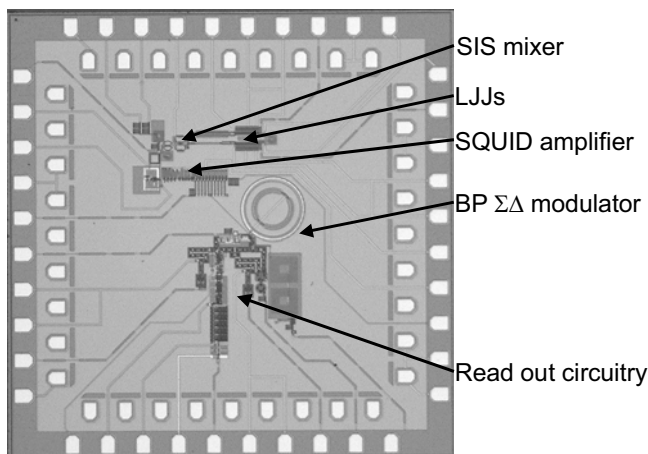


Fig. 2. The photo of front-end chip. See text for details.

For easy testability we are developing a self-contained spectrometer, e.g. no actual outside signal is investigated and this outside signal is modeled by an on-chip oscillator, very similar to the LO only with weaker coupling to mixer.

Unidirectional fluxon (flux quantum $\Phi_0 = h/2e$) propagation in a long Josephson tunnel junction (LJJ) is used as a way to achieve a practical and compact on-chip LO. A Josephson junction is defined as “long” when its physical length $L \gg \lambda_j$ and the width $W \ll \lambda_j$, where Josephson penetration depth λ_j is the characteristic dimension of an unperturbed fluxon. A fluxon in a long Josephson junction (LJJ) carries a magnetic flux equal to one flux quantum Φ_0 . A dc magnetic field H is applied in the plane of the junction. With increasing the external magnetic field, the screening current at the junction edge becomes unstable and forms a closed loop, which enters the interior of the junction. Fluxons are continuously generated at one junction end, and accelerated by the bias current toward the other end. Here the reflections generate a regular standing wave pattern resulting in emitted radiation. The oscillation frequency is described by the formula: $f = V_{dc} / \Phi_0 = u d \mu_0 H / \Phi_0$, where d is the magnetic thickness of the junction and μ_0 is the permeability free space. The average velocity u of fluxons is proportional to the bias current.

The oscillation frequency can be tuned over the wide range by changing the applied field, by varying the fluxon density in the junction, and by changing the bias current.

All circuits in this paper are fabricated using the standard HYPRES 3 μm 1 kA/cm² process⁹. Fig. 2 shows the layout of the chip that incorporates all front-end structures. The chip consisted of the following major parts: the LO in the form of long Josephson junction, SIS mixer, weakly coupled LJJ to model external signal, various transformers for better impedance matching of SIS mixer to LJJs, SQUID amplifier, and digital circuitry with bandpass delta-sigma modulator to test this structure as a whole. The LJJs/mixer circuitry is designed for better matching for the frequency of 350 GHz. The IF SQUID amplifier has been designed for the 1 GHz bandwidth. LO LJJ and weakly coupled LJJ have to be adjusted within 1 GHz difference around 350 GHz.

All components of the front-end chip have been tested. For the LO/SIS mixer structure, the current-voltage characteristic (I-V curve) of the LO, when a 7 mA current is applied through the control line, exhibited a pronounced flux-flow step at 0.75 mV. At the same time, the I-V curve of the SIS mixer irradiated by the LO, while its Josephson current is suppressed by current through control line and when LO is biased at flux-flow step, exhibits the photo-assisted tunneling step at hf_{RF}/e below the gap.

The main purpose for the SQUID amplifier on the front-end chip is to match low input impedance of bandpass modulator ($Z_{in} \ll 1 \Omega$) and high output impedance of SIS mixer ($Z_{out} \approx 50 \Omega$) with simultaneous filtering of all out of IF band signals. The realized amplifier consists of a front end and a power amplifier. The front-end is a simple two-junction voltage-mode SQUID to transform the input signal current into the stream of SFQ pulses. The pulses are amplified in power by passing over the Josephson transmission line (JTL) with exponentially increasing critical and bias currents of the Josephson junctions. The final stage of JTL and resistive-inductive network provide both the power gain and low-pass filtering in order to suppress the SQUID’s Josephson oscillations and to refine the amplified signal.

The output signal is the current through a load inductor, which is inductively coupled to the modulator. The single Josephson junction connected in series with the load acts as the signal limiter.

The resonance frequency of mixer-amplifier tank circuit is measured to be 1.5 GHz. The SQUID amplifier has the following experimentally measured parameters: critical current and normal state resistance per junction of front end SQUID are $I_c=40 \mu\text{A}$ and $R_N=4 \Omega$, SQUID inductance is 40 pH, mutual input inductance is 400 pH and input inductance is 5 nH providing the amplifier noise temperature $T_N=90 \text{K}$.

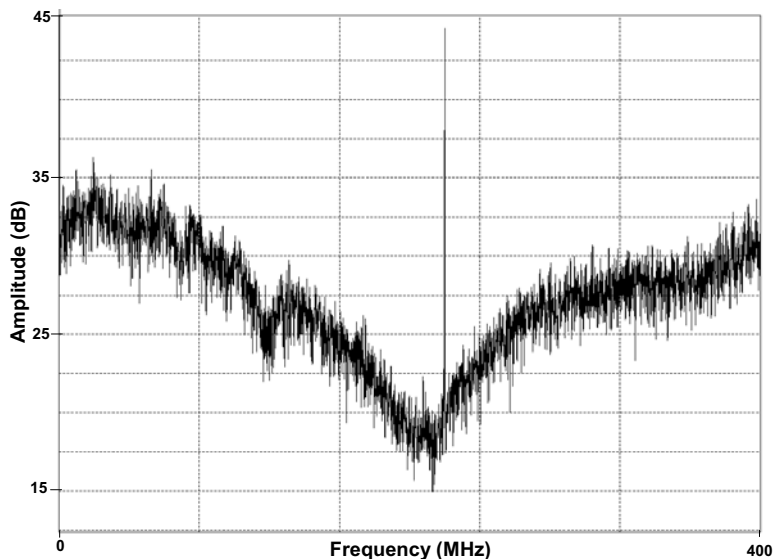


Fig. 3. Spectrum from bandpass delta-sigma modulator (1-bit digitizer) with clock signal at 800 MHz and input signal at 1020 MHz.

A first-order bandpass delta-sigma modulator with a center frequency of 1 GHz that used a lumped-element LC resonator is designed and fabricated on the front-end chip. The modulator uses implicit feedback – the switching of the clocked comparator automatically feeds $-\Phi_0$ back to the resonator – which is a fundamental advantage of superconductor delta-sigma modulators. In order to be able to verify performance of stand-alone front-end chip, the modulator is connected to read out digital circuitry, e.g., a high-speed output driver. The data from the modulator's output are converted to non-return-to-zero voltage-potential form, amplified and transferred to room temperature for additional amplification and processing.

Fig. 3 shows the measured spectrum of bandpass modulator when -20 dBm (-3 dB full scale) 1020 MHz input signal is sampled with 800 MHz clock. The undersampled spectrum clearly shows tone corresponding to 1020 MHz and expected noise shaping with dip of 15 dB in vicinity of 1 GHz.

4. Digital Signal Processing

The correlator circuit as the core component of our digital signal processor has been selected. The 128-channel autocorrelator that gives 8 MHz frequency resolution, e.g. appropriate for space-borne application has been designed and its correct operation has been verified. Our approach in design of 128-channel autocorrelator is to compose it from a 16-channel autocorrelator and 112-stage PRSR. The shift register should have number

of switches. By closing these switches data can be directed through or bypassing different digital delay lines, obtaining the data delay in increments of 16.

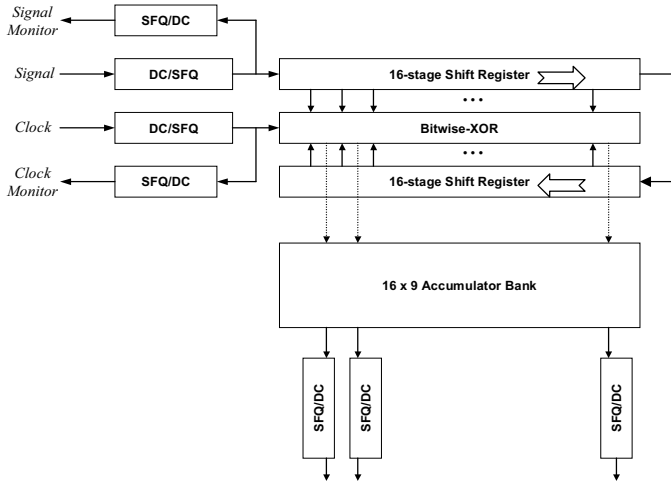


Fig. 4. The block diagram of 16-channel digital autocorrelator.

Fig. 4 shows the block diagram of 16-channel digital autocorrelator. The digital 16-channel autocorrelator forms a linear array with two main parts: digital delay lines with multipliers and an array of binary counters. The binary counters are composed of T flip-flop gates, outputting only the most significant bits. The individual components of the design - the circular shift register, XORs and T flip-flop gates are well known and have been reported to have very wide operating margins in many studies. Straightforward integration of these gates into an operational subsystem is possible only for the T flip-flop counters, due to their asynchronous mode of operation and unusually wide parameter margins. Integration of the XOR gates into the circular shift register is a much less trivial task, mostly due to numerous timing requirements.

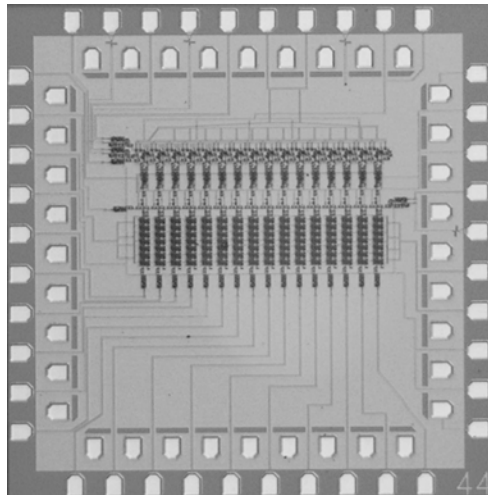


Fig. 5. The photo of 16-channel digital autocorrelator chip.

The main part of the autocorrelator is the digital delay line, which is based on a circular shift register with XOR multipliers built into every stage. The digital test at low speed is performed to verify the correct operation of a 32-stage circular shift register. The total number of D flip-flops in the shift register is 34:2 D flip-flops per each regular stage plus 2 in the “0-th” stage, where data makes a U-turn.

The 16-channel autocorrelator has been fabricated (the layout is shown in Fig. 5) and successfully tested using OCTOPUX test system capable of performing exhaustive low speed (500 Hz) tests of large digital and analog circuits.

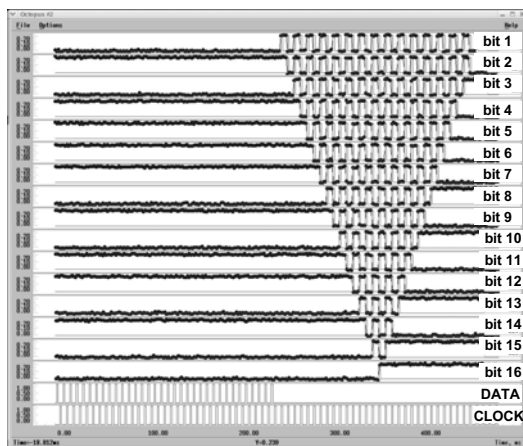


Fig. 6. Low-frequency testing of the 16 channel autocorelator. For the data and clock inputs each rectangular pulse corresponds to an SFQ pulse.

Fig. 6 shows the correct operation of the 16 channel autocorrelator without accumulator bank for the test sequence when a train of $2 \times 16 + 2 = 34$ ‘1’s (signal “DATA” in Fig. 6) is loaded into the circular shift register. High as digital ‘1’ and low as digital ‘0’ are interpreted. The correct operation of all 16 XOR gates (outputs O1-O16) for all possible combinations of inputs (“00”, “10”, “01”, “11”), as well as correct operation of the circular shift register under full load is demonstrated.

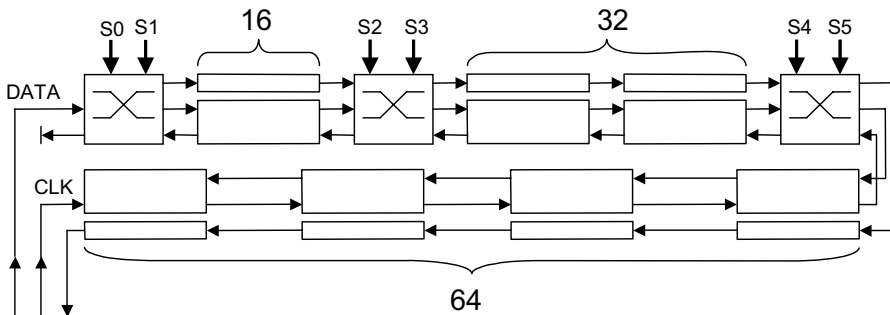


Fig. 7. The block diagram of programmable delay 112-stage shift register.

Fig. 7 shows the block diagram 112-bit PRSR. This shift register includes 112 stages divided into three chunks of 16, 32 and 64 stages together with 6 switches S0-S5. It employs more robust counter-flow design¹⁰, e.g. the stream of data and clock pulses flow in opposite directions. By applying DC current to different combination of the switches

we are able to choose any delay from 0 to 112 in increments of 16. The 112-stage PRSR has been fabricated and a photo of the chip is presented in Fig. 8.

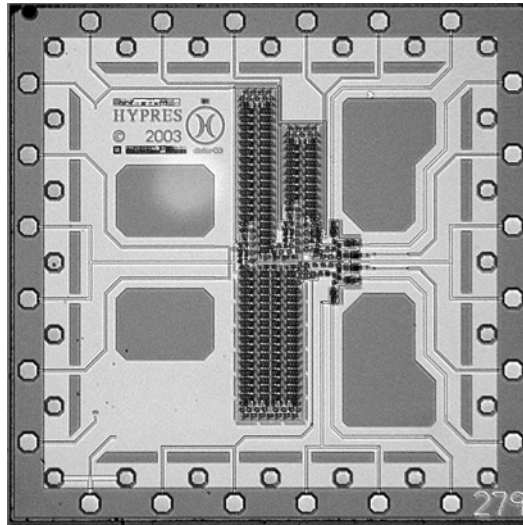


Fig. 8. The photo of 112-bit programmable shift register chip.

The operation of the shift register has been successfully verified by using OCTOPUX. As an example, fig. 9 presents test results for the 112-bit PRSR with correct operation of the shift register with switches S0, S3 and S5 closed while switches S1, S2 and S4 are opened, showing the delay of data at the output for 16 clock cycles. Fig. 9 shows the following three groups of data traces: data and clock inputs – inputs that have been generated by OCTOPUX and sent to the chip, data and clock monitors – traces experimentally measured immediately after appropriate entrances to the chip, and clock and data outputs- traces measured after clock and data propagated through all 112 stages of shift register. The data output exhibits the correct 16-clock cycles delay.

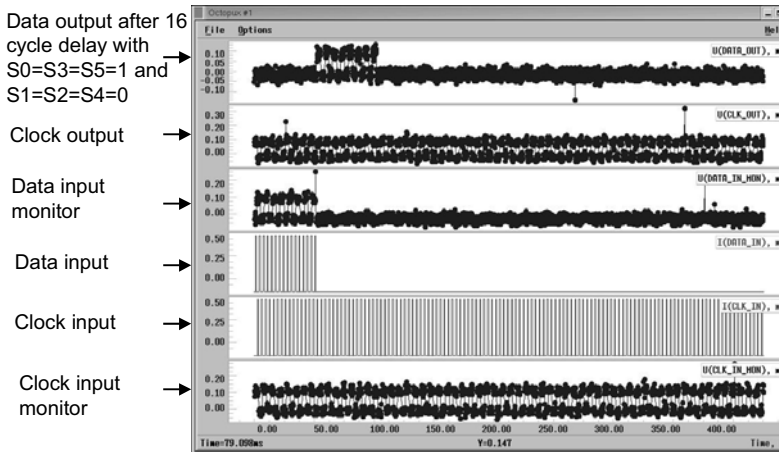


Fig. 9. Test results for the 112-bit PRSR with 16 clock cycles delay.

The correct performance of 16-lag autocorrelator and 112-lag PRSR has been verified. Their high-speed operation has been already realized before: autocorrelator at 11 GHz¹¹ and more complex shift register at 19 GHz¹⁰. After integration, our DSP circuit is expected to operate at slightly lower speed, still sufficient for intended applications – to acquire spectra of slow changing signals.

5. Packaging

A key element of the spectrometer package is the cryocooler – a cryogenic refrigerator needed to maintain the superconducting circuits at these low operating temperatures. Historically, superconducting systems required cooling with liquid helium, rendering its use expensive and inconvenient in terms of cryogen logistics. Recently, reliable closed cycle refrigerators (cryocoolers) have become commercially available. These are turnkey electrical machines with no liquid cryogenics, analogous to home freezers and air-conditioning units, requiring only standard electrical power to deliver continuous operation for years. HYPRES has sold commercial SCE systems mounted on a commercial-off-the-shelf (COTS) cryocooler, which have exhibited extended performance superior to their liquid-He cooled counterparts. The technology for producing these cryocoolers has evolved over several decades, and recent developments now enable reliable products of unprecedented efficiency and reliability. Products utilizing superconductor materials for analog signal processing are commercially deployed and several hundred units have demonstrated over 3.5 Million hours of operation with mean-time-between-failures (MTBF) exceeding 99 years. Fig. 10 shows a concept sketch of a two-channel (capable of screening for the presence of chemical and biological agents at two different locations) spectrometer in a cryocooler fit for a standard 19" rack. The number of channels can be extended to as many as ten.

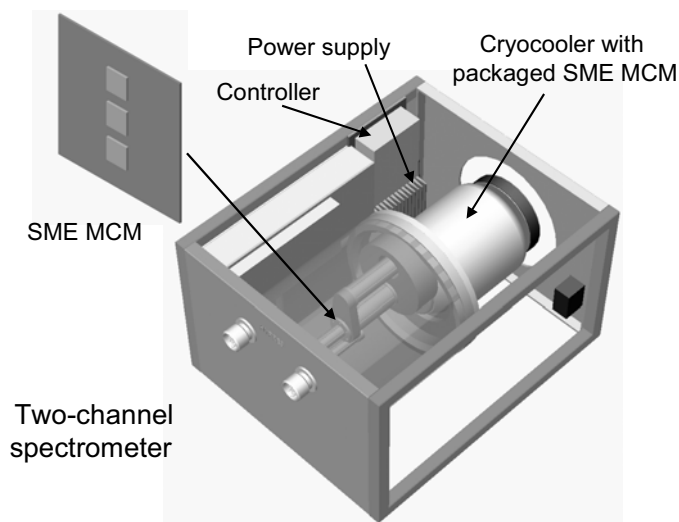


Fig. 10. The concept sketch of a two-channel spectrometer packaged in the cryocooler.

6. Conclusions

A compact ultrasensitive wideband superconducting mm/submm integrated digital spectrometer for chemical and biological agent detection is being developed. In addition, this spectrometer may be used in radio-astronomical research and remote monitoring of the Earth atmosphere. Correct performance of all integrated spectrometer analog and digital components, such as local oscillator/SIS mixer structure, IF SQUID amplifier, bandpass delta-sigma modulator, autocorrelator and programmable delay shift register have been successfully verified.

Assembled on a multi-chip module and packaged on COTS cryocooler the complete spectrometer offers integration of thin film analog components such as a quasioptical antenna with mixer, superconducting local oscillator and an IF SQUID amplifier together with superconducting digital circuitry.

7. Acknowledgments

This work was supported in part by Missile Defense Agency contract no. DASG60-03-C0007.

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