Sub-THz CMOS Molecular Clock with 43ppt Long-Term Stability Using High-Order Rotational Transition Probing and Slot-Array Couplers

Cheng Wang, Xiang Yi, Mina Kim, Ruonan Han
Massachusetts Institute of Technology, Cambridge, MA
Outline

• Background
• High-order locking for long-term stabilization
• Architecture and circuit design
• Measurement results
• Conclusions
Ultra-Stable, Miniaturized Clocks

Synchronization of high-speed radio access networks

- 5G massive MIMO $\rightarrow \sigma_t < 65\text{ns}$
- Precise positioning $\rightarrow \sigma_t < 10\text{ns}$
- 1-min holdover $\rightarrow \Delta f < 10^{-10}$

Precise timing for underwater oil exploration

- Temp. variation $\rightarrow \Delta f < 10^{-9}$
- Deployment time $\rightarrow \text{Weeks}$
- DC Power $\rightarrow \sim 100\text{mW}$

[researchsnipers.com]
Comparison of Portable Clocks

<table>
<thead>
<tr>
<th></th>
<th>Oven compensated crystal oscillator (OCXO)</th>
<th>Chip-scale atomic clock (CSAC)</th>
<th>Chip-scale molecular clock (CSMC) (This work)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stability</td>
<td>(\sim 10^{-10}@10^3 \text{s}) 🙁</td>
<td>(\sim 10^{-11}@10^3 \text{s}) 🎉</td>
<td>(\sim 10^{-11}@10^3 \text{s}) 🎉</td>
</tr>
<tr>
<td>Power</td>
<td>(~1\text{W}) 🙁</td>
<td>(~100\text{mW}) 🎉</td>
<td>(~100\text{mW}) 🎉</td>
</tr>
<tr>
<td>Cost</td>
<td>(~$100) 🎉</td>
<td>(~$1000) 😞</td>
<td>(~$10) 🎉</td>
</tr>
</tbody>
</table>

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Rotational Spectra of Polar Gaseous Molecules

EM field

E or M dipole

MW photon

hν

Polar gaseous molecules

Quantized rotational states

J=1
J=2
J=3
J=4
J=5
J=6
J=7

Photon absorption \( \rightarrow \) state transition \( (J \rightarrow J+1) \)

Rotational spectra observed in WG gas cell

E/M torque \( \rightarrow \) molecular rotation

\( f_{FWHM} \)

\( Q = \frac{f_0}{f_{FWHM}} \)

\( \sim 2 \times 10^5 \)
Wavelength Modulation Spectroscopy (WMS)

- \( K \): “open” \( \rightarrow \) rotational spectrometer

\[
V_{WM}(t) = A(t) \cdot \sin[2\pi f_p t + \Delta f \cdot \sin(2\pi f_m t + \theta_0)]
\]

- \( f_m \): Modulation freq.
- \( \Delta f \): Freq. deviation

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High Order Harmonics of $f_m$

- Rotational spectral line
- Output of THz detector

$A^2(t)$

$f_p < f_0$

Spectrum (dB)

$f_p = f_0$

Spectrum (dB)
High Order Harmonics of $f_m$
Multi-Order Dispersion Curves

N\textsuperscript{th} order dispersion curve \approx N\textsuperscript{th} order derivative

Rotational spectral line

Spectrum of $A^2(t)$

Transmission (%)

$V_{LK,1}$

$V_{LK,2}$

$V_{LK,3}$

$V_{LK,4}$

1\textsuperscript{st} order

2\textsuperscript{nd} order

3\textsuperscript{rd} order

4\textsuperscript{th} order

N\textsuperscript{th} order dispersion curve \approx N\textsuperscript{th} order derivative

$f_{FWHM}$

$f_f - f_p$

$f_p < f_0$

$f_{m}$

$\frac{1}{f_m}$

$t$

Instant. freq. of $V_{WM}(t)$

Sweep $f_p$
Multi-Order Dispersion Curves

Odd order curves → zero-crossing point

Rotational spectral line

Spectrum of $A^2(t)$

Transmission (%)

$1/f_m$ → $0$

$1/f_{FWHM}$

$0$ $f_p = f_0$

$\Delta f$

Sweep $f_p$

$0$ $f$

$1/f_m$

Instant. freq. of $V_{WM}(t)$

$V_{LK,1}$ $V_{LK,2}$ $V_{LK,3}$ $V_{LK,4}$

$1^\text{st}$ order $2^\text{nd}$ order $3^\text{rd}$ order $4^\text{th}$ order

$f_p - f_0$ (MHz)

$0$ $2$ $4$

$0$ $2$ $4$ $0$ $2$ $4$ $0$ $2$ $4$
Molecular Clock Locking to Spectral Line Center

Allan deviation:

$$\sigma_y = \frac{V_n}{\sqrt{2T \cdot K_r \cdot f_0}} \approx \frac{N_0}{\sqrt{T \cdot Q \cdot SNR}}$$

$$\tau - \text{Avg. time}$$

Zero-crossing point:
- $K_r$: Response, [V/Hz]
- $V_n$: Noise, [V/\sqrt{\text{Hz}}]

$$SNR = \frac{V_{\text{error,max}}}{V_n}$$

- $K$: “closed” $\rightarrow$ Lock to zero-crossing point
Proof-of-Concept: The 1st CSMC Prototype

- 231.061GHz line of OCS
- 1st order dispersion curve
- Frequency stability: \( \sigma_y = 3.8 \times 10^{-10} @ \tau = 10^3 \text{s} \)
- 66mW DC power.
Frequency Stability of Molecular Clock

Short term

Medium term

Long term

VCXO noise

Allan deviation, $\sigma_y$

$\sigma_y \approx \frac{N_0}{\sqrt{T \cdot Q \cdot SNR}}$

Drift due to baseline tilting

- This work: High order locking

Temperature dependency

Drift due to Magnetic field

Drift due to Electrical field

$1 \quad \text{GBW}$

10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2} 10^{3} 10^{4} \tau \ (s)$
Asymmetric Line Profile due to Baseline Tilting

- Symmetric in theory
- THz transceiver response
- Gas cell response
- Measured in reality

Rotational spectral line + Baseline tilting = Asymmetric line profile
1st Order Dispersion Curve w/ Baseline Tilting

1st order dispersion curve

- Invariant zero-crossing point under PVT

Offset voltage $V_{Offset}$

- $V_{offset}$ is PVT dependent

Long-term clock drift

- How to deal with varying zero-crossing point?

$T_{Low}$
$T_{Medium}$
$T_{High}$

$V_{LK,1}$

Baseline tilting

1st Order Dispersion Curve w/ Baseline Tilting

1st order dispersion curve

- Invariant zero-crossing point under PVT

Offset voltage $V_{Offset}$

- $V_{offset}$ is PVT dependent

Long-term clock drift

- How to deal with varying zero-crossing point?
High Order Dispersion Curve w/ Baseline Tilting

- Invariant zero-crossing point under PVT
- Eliminated by high order derivative, \( V_{\text{offset}} \approx 0 \)
- Invariant zero-crossing point under PVT
Idea: CSMC with High-Order Locking

- Simulation: 0.1dB/GHz baseline tilting → a frequency drift of:
  - $5 \times 10^{-9}$ for 1st order locking
  - $3 \times 10^{-10}$ for 3rd order locking

- This work: a chip-scale molecular clock (CSMC) locking to high order dispersion curve
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System Architecture

THz detector

VGA

4N⋅fm

A2(t)

WM

V_m(f_m=100kHz)

60MHz

PLL2

231.06GHz

VCXO

PLL1

GDC

VLK,N

XTAL

f_out: 60MHz

f_p=231.06GHz

V_{WM}(t)

OCS molecules

Gas cell

On-chip Coupler

Off-chip HRLKD

Trans(%) A2(t) f_p(t)

t

f_p(t)
TX: 231GHz Cascaded Two-Stage PLL

- Freq. tunability: ~1% of line width $f_{FWHM}$
- 27GHz (12%) bandwidth for line coverage
- Precise wavelength modulation (WM)
  - $\Delta f/f_p \approx 10^{-5}$ ($\Delta f \approx 2.5$MHz, $f_p = 231.06$GHz)
TX PLL2: 57.77GHz VCO and 231GHz Quadrupler

- Varactor 1: highly-sensitive for large PLL bandwidth
- Varactor 2: low sensitivity for wavelength modulation
  - \( KVCO_{\text{Varactor 1}} / KVCO_{\text{Varactor 2}} \approx 10^3 \)
TX: Wavelength Modulator (WM)

- 100kHz differential output voltage
- 3-bit Δf control
- 0.6° phase control
- Low distortion: spur < -55dB
RX: THz Detector and VGA

- Sub-threshold NMOS pair → low noise THz square-law detector
- 2-stage variable gain amplifier
  - 65dB max gain / 10-bit control
  - AC coupled / monolithic integrated
RX: Harmonic Rejection Lock-in Detector (HRLKD)

- Convert $N^{th}$ harmonic of $f_m$ to DC
- Harmonic rejection of ref. clock $f_{\text{ref}}$ for low interference and noise-folding
- Reduce flicker noise at DC output
RX: Harmonic Rejection Lock-in Detector (HRLKD)

- DC offset $V_p - V_n \approx 10\mu V$ (1µV change $\rightarrow 10^{-10}$ drift)

- Harmonic rejection $> 80$dB

- Reduced DC flicker noise
Chip-to-Waveguide Coupler

E-plane quartz probe
[C. Wang, et al., JSSC, 2018]

Dielectric resonator
[D. L. Cuenca, et al., EuMIC, 2017]

Integrated dipole coupler
[H. Song, et al., MWCL, 2016]

• Conventional designs
  • Costly external components
  • Special process/wafer thinning
  • Insufficient TRX isolation
Slot Array Coupler: Architecture

- Radiates downward into waveguide aperture through Si-substrate
- No external components
- No wafer thinning
Slot Array Coupler: Simulated Results

- Simulated loss = 5.2 dB
- $BW_{3dB} = 21\%$
- 60 dB simulated TX/RX isolation
- $10^{-9}$ drift by 60 dB isolation (removable w/ calibration)
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Chip Photo and Packaging

- TSMC 65nm CMOS process.
Measured RF Power and Phase Noise of TX

- $P_{RF} = -9.4\, \text{dBm}$ w/ slot array coupler
- PLL bandwidth: 27GHz (12%)
- Phase noise : $-81.5\, \text{dBc}/\text{Hz}@1\, \text{MHz}$
- PM-to-AM noise $\rightarrow SNR_{PN} = 84\, \text{dB}$

![Graph showing measured and simulated TX power with slot array coupler.](image)

![Graph showing phase noise of PLL1: 3.21GHz and PLL2: 231.06GHz.](image)
Measured WMS Spectrum and RX Performance

\[ f_0 = 231.06\text{GHz}, \quad f_m = 100\text{kHz} \]

- Spectrum of TX probing signal with wavelength modulation
- NEP of RX w/ slot array coupler: 62.8 pW/√Hz at \( f_m = 100\text{kHz} \)
Measured Dispersion Curves and Allan Deviation

- 1\textsuperscript{st} order curve: SNR = 84dB
- \( V_{\text{Offset}} = 1.1\text{mV} \)

- 3\textsuperscript{rd} order curve: SNR = 66dB
- \( V_{\text{Offset}} = 4.3\mu\text{V} \) (256× smaller)
Measured Allan Deviation by 3\textsuperscript{rd} Order Locking

- Allan deviation: $\sigma_y = 3.2 \times 10^{-10} @ \tau = 1\text{s}$, $4.3 \times 10^{-11} @ \tau = 10^3\text{s}$
Measured Temperature and Magnetic Sensitivity

- Drift $< \pm 3 \times 10^{-9}$ in $27\sim65$ °C w/ 2$^{\text{nd}}$ order temperature compensation
- Drift $< \pm 2.9 \times 10^{-12}$/Gauss w/o magnetic shield in CSAC
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## Performance Comparison Table

<table>
<thead>
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<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Mechanism</td>
<td>OCXO</td>
<td>$^{133}$Cs CSAC</td>
<td>$^{133}$Cs CSAC</td>
<td>$^{16}$O$^{12}$C$^{32}$S MC</td>
<td>$^{16}$O$^{12}$C$^{32}$S MC</td>
</tr>
<tr>
<td>Cost</td>
<td>Medium</td>
<td>High</td>
<td>High</td>
<td>Low</td>
<td>Low</td>
</tr>
<tr>
<td>Freq. (GHz)</td>
<td>0.06</td>
<td>4.6</td>
<td>4.6</td>
<td>231.061</td>
<td>231.061</td>
</tr>
<tr>
<td>Harmonics</td>
<td>N/A</td>
<td>1$^{\text{st}}$ order</td>
<td>1$^{\text{st}}$ order</td>
<td>1$^{\text{st}}$ order</td>
<td>3$^{\text{rd}}$ order</td>
</tr>
<tr>
<td>$\sigma_y (\tau = 10^0 \text{s})$</td>
<td>3.0×10$^{-11}$</td>
<td>3.0×10$^{-10}$</td>
<td>8.4×10$^{-11}$</td>
<td>2.4×10$^{-9}$</td>
<td>3.2×10$^{-10}$</td>
</tr>
<tr>
<td>$\sigma_y (\tau = 10^3 \text{s})$</td>
<td>4.0×10$^{-11}$</td>
<td>1.0×10$^{-11}$</td>
<td>0.8×10$^{-11}$</td>
<td>3.8×10$^{-10}$</td>
<td>4.3×10$^{-11}$</td>
</tr>
<tr>
<td>Temp. Drift $^a$</td>
<td>±5.0×10$^{-9}$</td>
<td>±5.0×10$^{-10}$</td>
<td>&lt;±1.0×10$^{-9}$</td>
<td>N/A</td>
<td>±3.0×10$^{-9}$</td>
</tr>
<tr>
<td>Mag. Sens. $^b$</td>
<td>N/A</td>
<td>±9.0×10$^{-11}$</td>
<td>N/A</td>
<td>N/A</td>
<td>±2.9×10$^{-12}$</td>
</tr>
<tr>
<td>$T_{\text{start-up}}$ (s)</td>
<td>120</td>
<td>180</td>
<td>N/A</td>
<td>&lt;1</td>
<td>&lt;1</td>
</tr>
<tr>
<td>$P_{\text{DC}}$ (mW)</td>
<td>600</td>
<td>120</td>
<td>60</td>
<td>66</td>
<td>70</td>
</tr>
</tbody>
</table>

a. Measured temp. range: [1]: -20~70°C; [2], [3]: -10~70°C; This Work: 27~65°C;

b. Unit: Gauss$^{-1}$.

Acknowledgement

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• We appreciate the help from Qingyu (Ben) Yang on the experiments.
Demo Session 1

Chip Scale Molecular Clock
Sub-THz CMOS Molecular Clock with 43 ppt Long-Term Stability Using High-Order Rotational Transition Probing and Slot Array Couplers