OPTIMAL SPECTRAL RANGE AND OPERATION MODE FOR TRACE MOLECULE DETECTION WITH DL

A.I.Nadezhdinskii

NSC of A.M.Prokhorov General Physics Institute of RAS

Optimization of Tunable Diode Laser based systems for trace molecule detection is of great importance for different applications. System optimization approach has to take into account physical properties of all system elements: DL, photo-detector, optical scheme, object of interest, etc. As result, for many molecules S/N ratio is higher in near IR spectral range where overtones and combination bands are located in comparison with fundamentals in mid IR. Comparison of quantum and thermal detectors is given. History of diode laser operation modes will be considered and their new generation with respect to diode laser physical properties is presented.

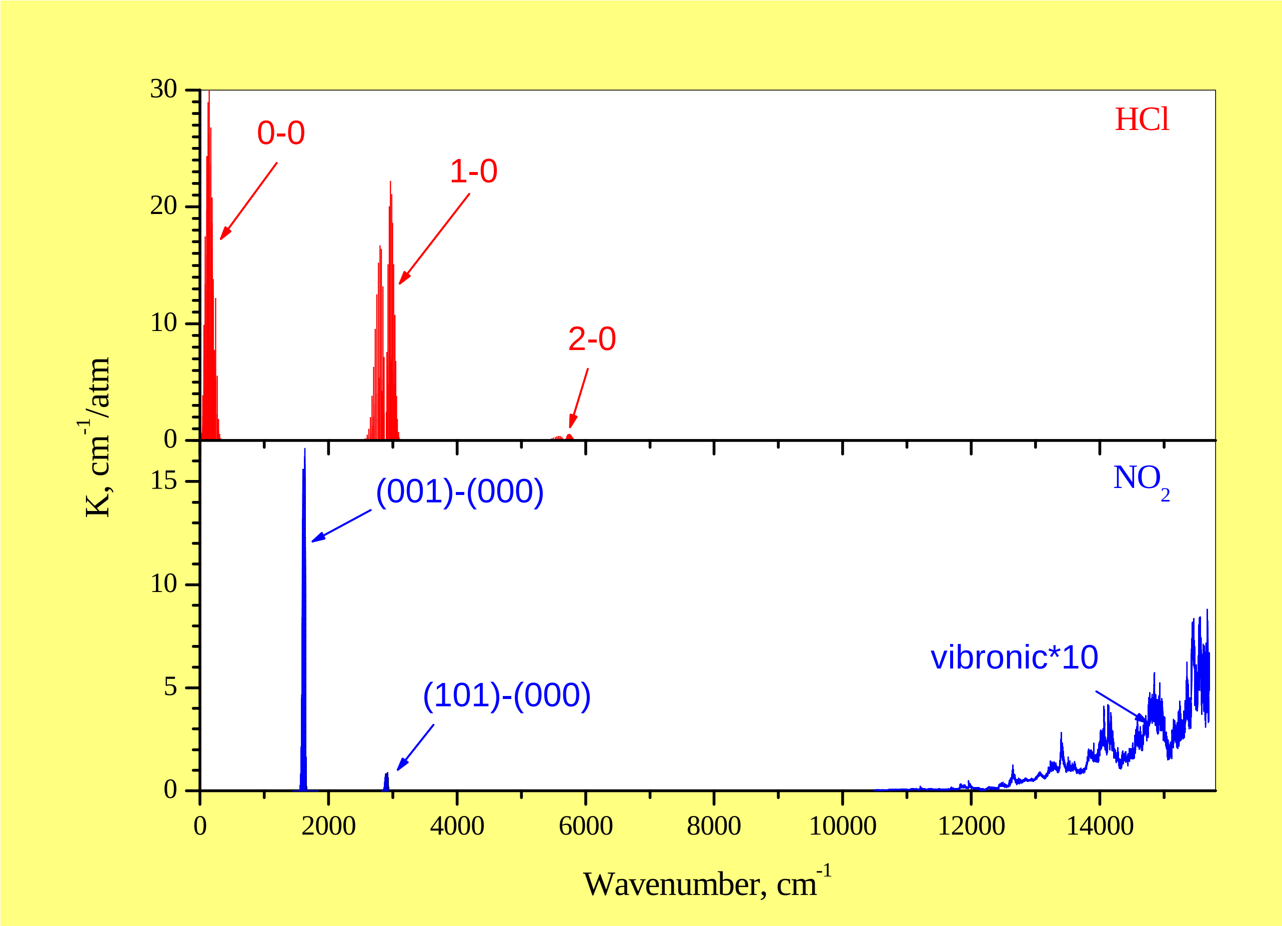
OPTIMAL SPECTRAL RANGE AND OPERATION MODE FOR TRACE MOLECULE DETECTION WITH DL

A.I.Nadezhdinskii

NSC of A.M.Prokhorov General Physics Institute of RAS

Optimization of Tunable Diode Laser based systems for trace molecule detection is of great importance for different applications. System optimization approach has to take into account physical properties of all system elements: DL, photo-detector, optical scheme, object of interest, etc. As result, for many molecules S/N ratio is higher in near IR spectral range where overtones and combination bands are located in comparison with fundamentals in mid IR. Comparison of quantum and thermal detectors is given. History of diode laser operation modes will be considered and their new generation with respect to diode laser physical properties is presented.

Molecular Spectra

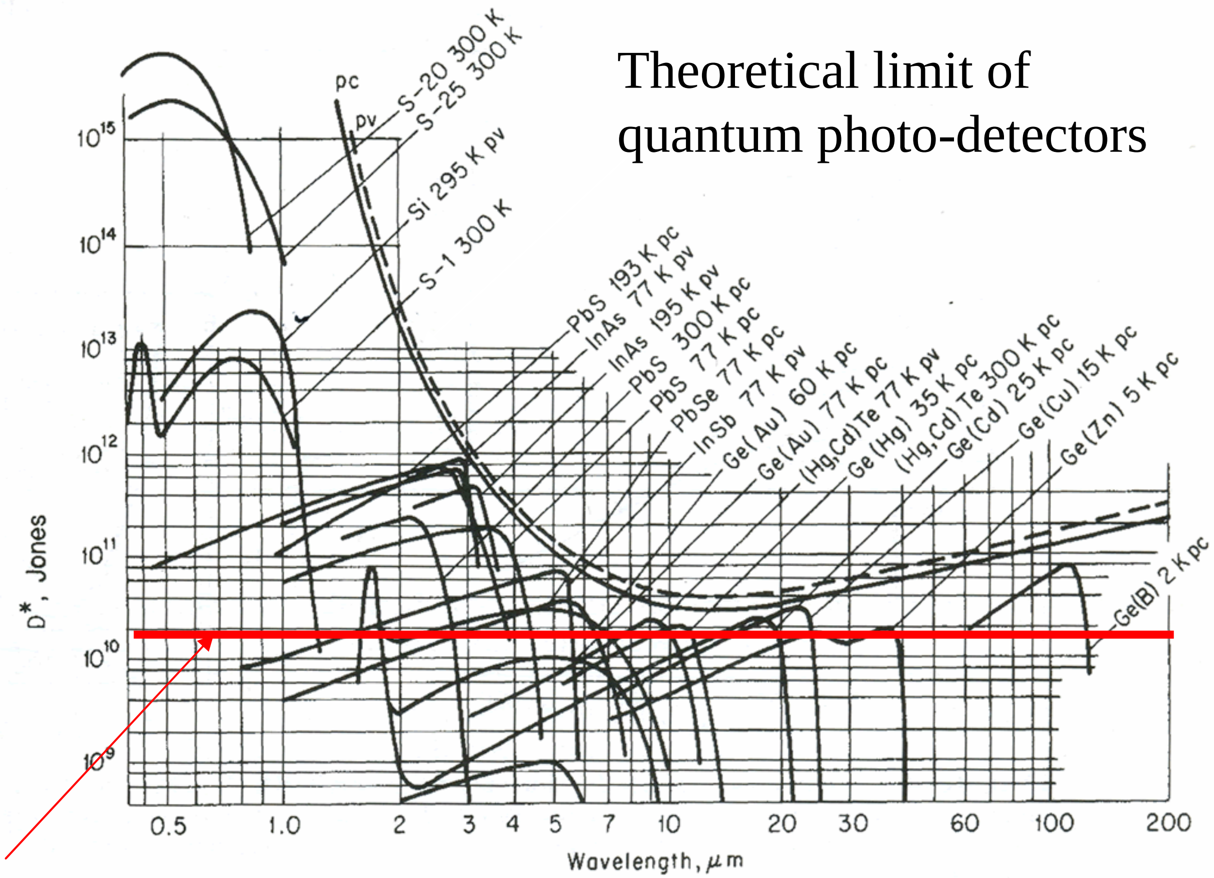


Different types of molecular absorption bands are using for trace molecule detection.

Traditionally fundamentals in mid IR are considered as the best candidates because of the highest absorption

Photo Detector Sensitivity

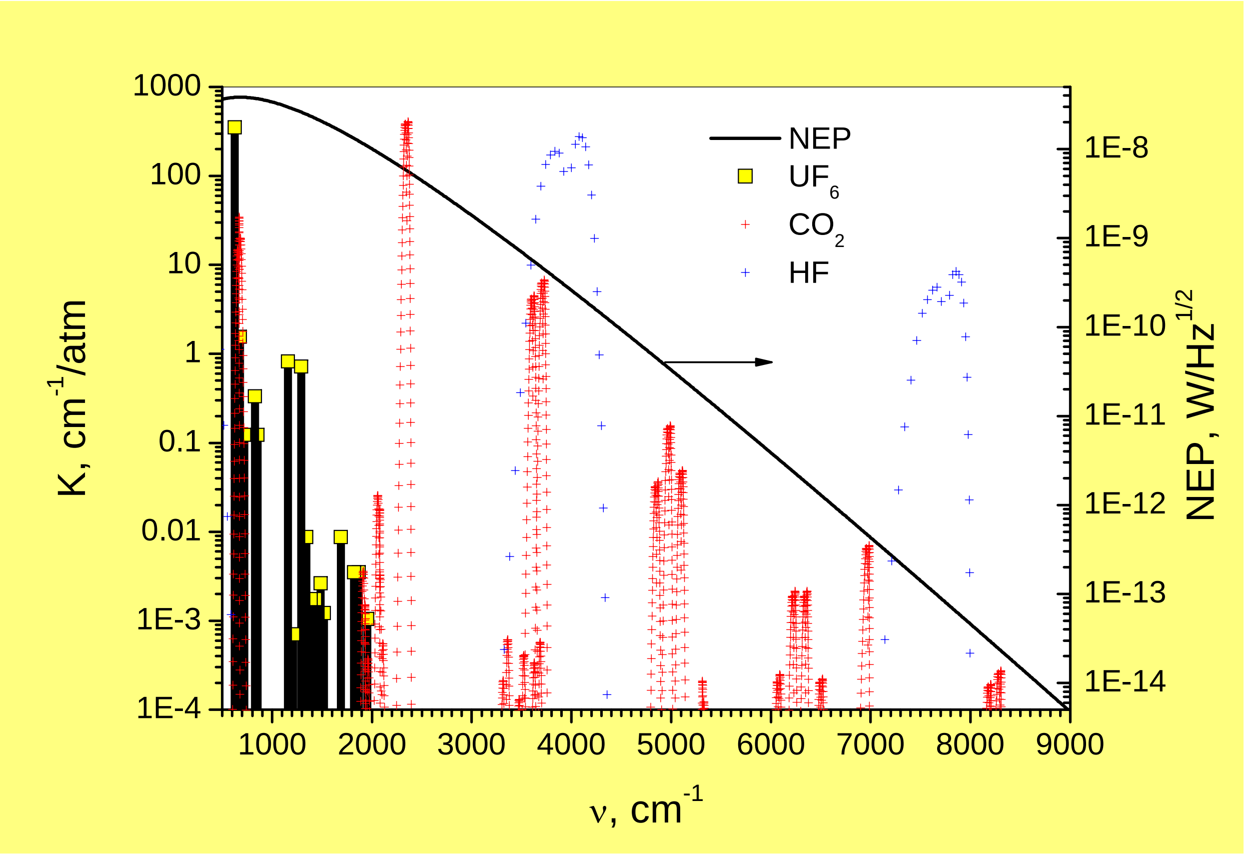
Theoretical limit of
quantum photo-detectors



Theoretical limit of thermal
photo-detectors

Molecules and Photo Detectors

Molecules can be classified into 3 main groups with respect to their Born-Oppenhimer parameter (root ratio of electron mass m to effective mass of normal vibration - M).

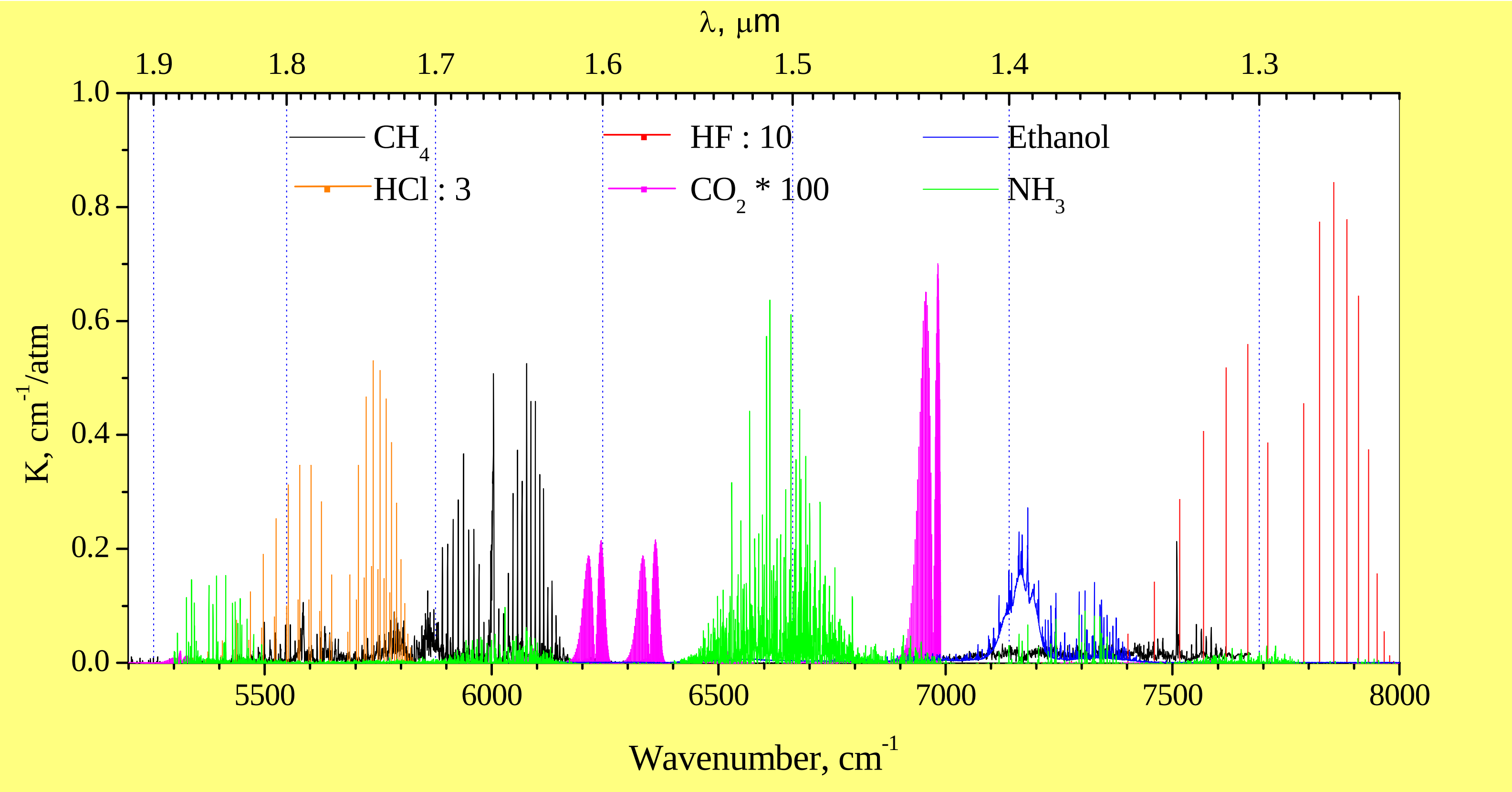


1. M~1 (Molecules with H – bond).
2. M~10 (C-O, N-O, …)
3. M~100 (UF_6, OsO_4, C_6H_6, …)

Comparison between absorption spectra of representatives of three molecular groups and photo-diode NEP (Noise Equivalent Power).

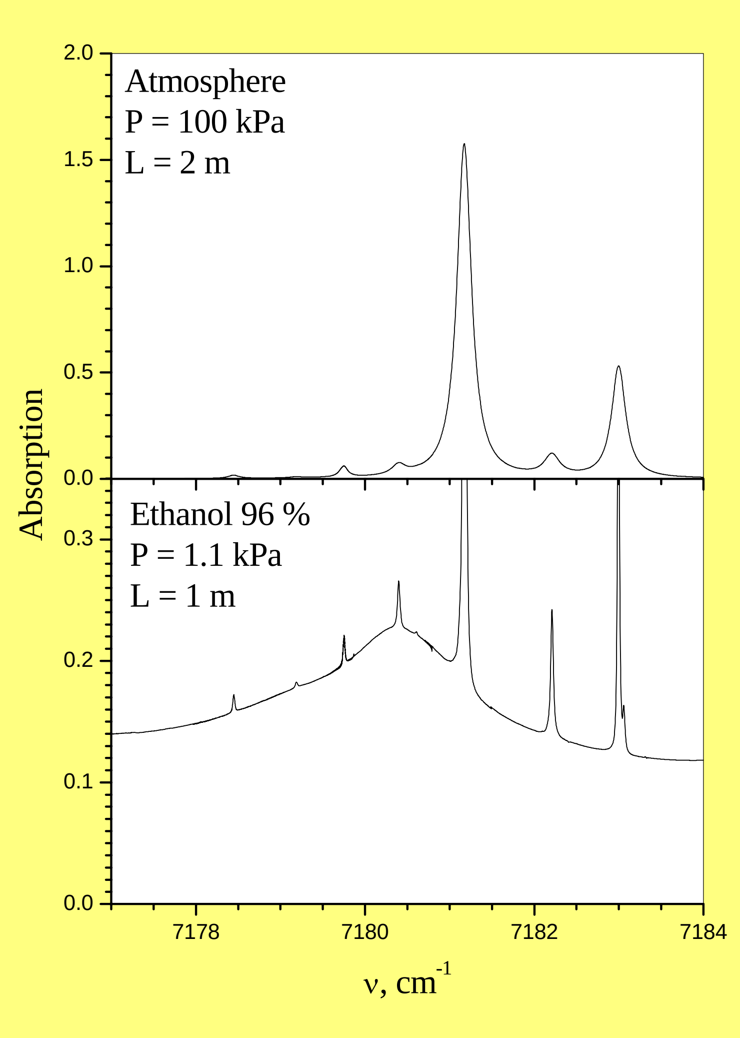
For many molecules S/N ratio is higher in near IR spectral range where overtones and combination bands are located.

Spectra of Several Molecules in Near Infrared Spectral Range



- Practically all molecules have absorption bands between 1 and 2 μm.
- Bands position are representative for molecular bonds such as C-H, O-H, N-H, etc.
- This spectral range is eye - safety

Spectral Lines Shapes



Absorption spectra of ethanol and water vapor near 1.39 μ

Atmosphere broadened water lines (top); ethanol vapor broad spectrum and Doppler water lines (bottom)

Taking into account spectral width of spectral features following classification can be proposed for trace molecule detection:

1. Low pressure: spectral lines with Doppler FWHH ~ 3 10^{-3} – 3 10^{-2} cm^{-1}
2. Atmosphere pressure: broadened spectral lines with FWHH ~ 0.1 cm^{-1}
3. Broadband absorber: FWHH ~ 1–10 cm^{-1}

For all three cases different strategies have to be selected to achieve highest sensitivity.

For optimal strategy : DL quantum noise limited sensitivity (see separate poster) was achieved for all three spectral features types.

Generation #1 of TDLS Operation Mode

To achieve high sensitivity averaging of data sets is necessary.
Due to statistical theory there are two possible ways of averaging: averaging over time and realizations averaging. For Markov random process (stationary, normal noise) both approaches will give the same result. The simplest one was time averaging and slow frequency tuning to obtain spectrum. It was used in generation #1 of TDLS operation mode.

Generation #1	Averaging over time, then slow frequency tuning	Harmonic excitation current modulation and signal 2f detection. Pulse-periodical DL operation and signal strobe integration

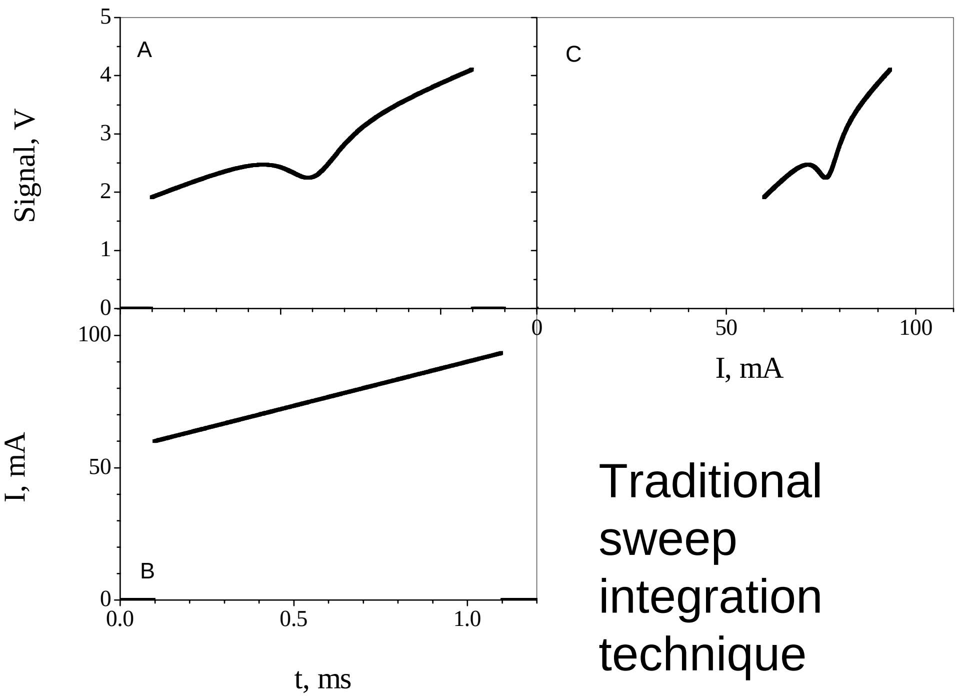
For non-Markov processes (Flicker noise, drift) typical for TDLS only one of approaches mentioned above is effective: quick signal recording and averaging over realizations. We proposed this approach more than decade ago and followed it in our activity.

Term ***“QUICK”*** depends on relative value of different noise mechanisms.

Generation #2 – Sweep Integration

Commercially available transient recorders in mid 80-th gave ability to record signal waveform and inverted generation #2 of TDLS operation mode – sweep integration.

Generation #2	Traditional sweep integration	Pulse-periodical DL operation and registration of each pulse. Averaging over realizations.



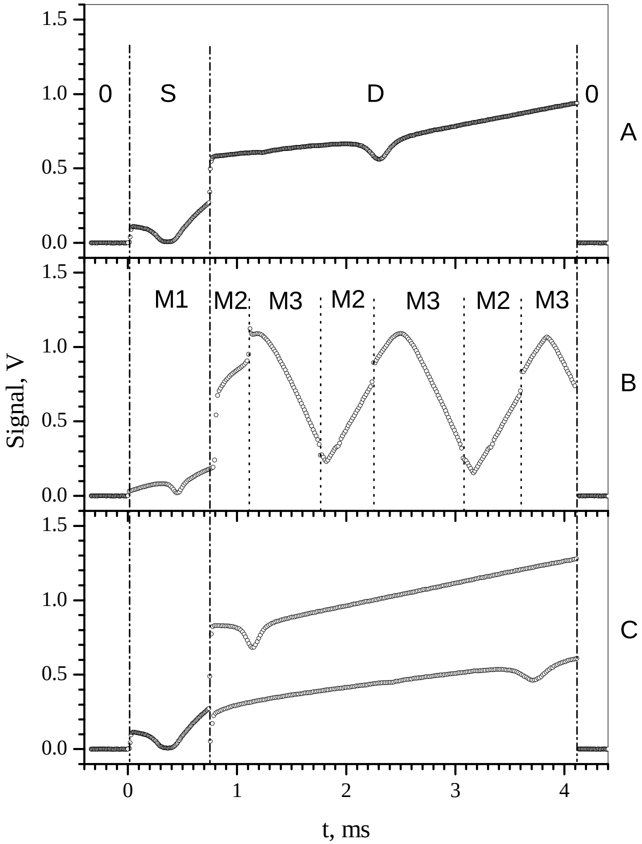
Traditional sweep integration technique

There are some variation of this approach. Main difference is method of signal filtering. 2f technique uses filtering in time domain.
As recorded signal is signal in DL frequency domain we are using optimal filter based on spectral line shape and dominant noise properties.
What means term ***"QUICK".***
For DL fundamental properties limited sensitivity (see separate poster) it means less than 300 mksec. If PD noise dominates it can be around 1 sec.

Generation #3

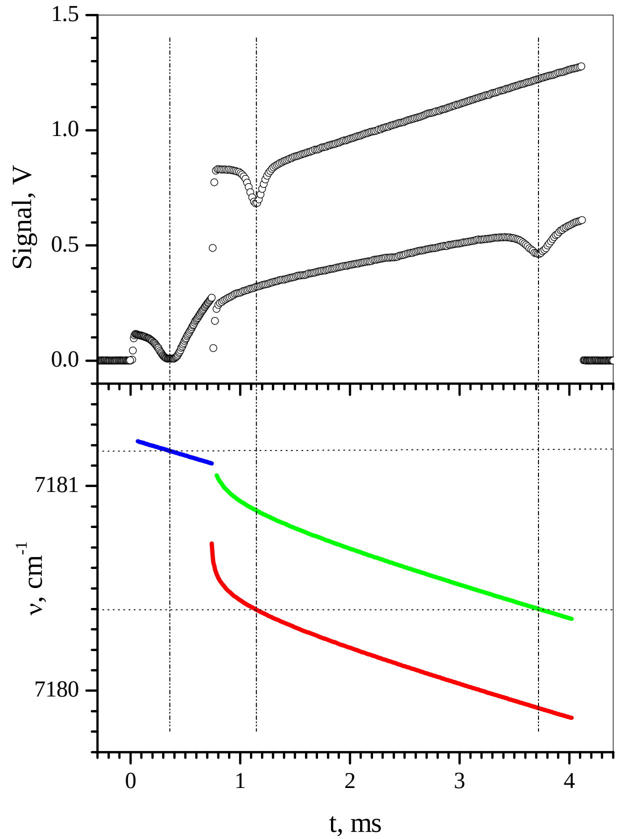
Commercially available today DAQs give additional ability to generate special excitation current waveform for optimal system operation.

Generation #3	Special excitation current waveform	Pulse-periodical DL operation with special excitation current waveform. Each pulse registration. Averaging over realizations.

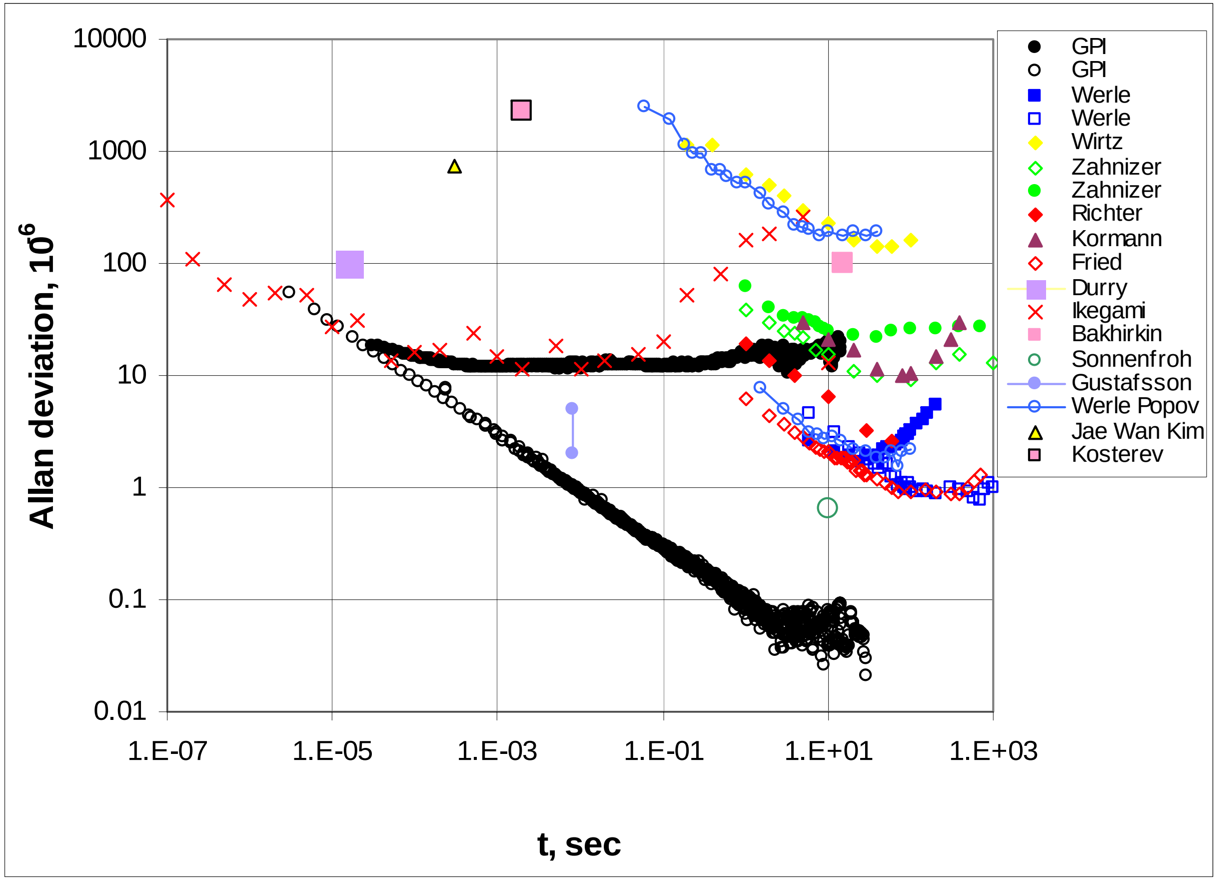


Left - examples of TDLS operation modes; 0 – DL current below threshold, S and D – regions used for stabilization and analytical purposes.

Right - recorded signal (top) and DL frequency tuning (bottom) for one of the operation modes in use. *It looks like two frequencies DL operation with tuning.*



Generation #3 in Use



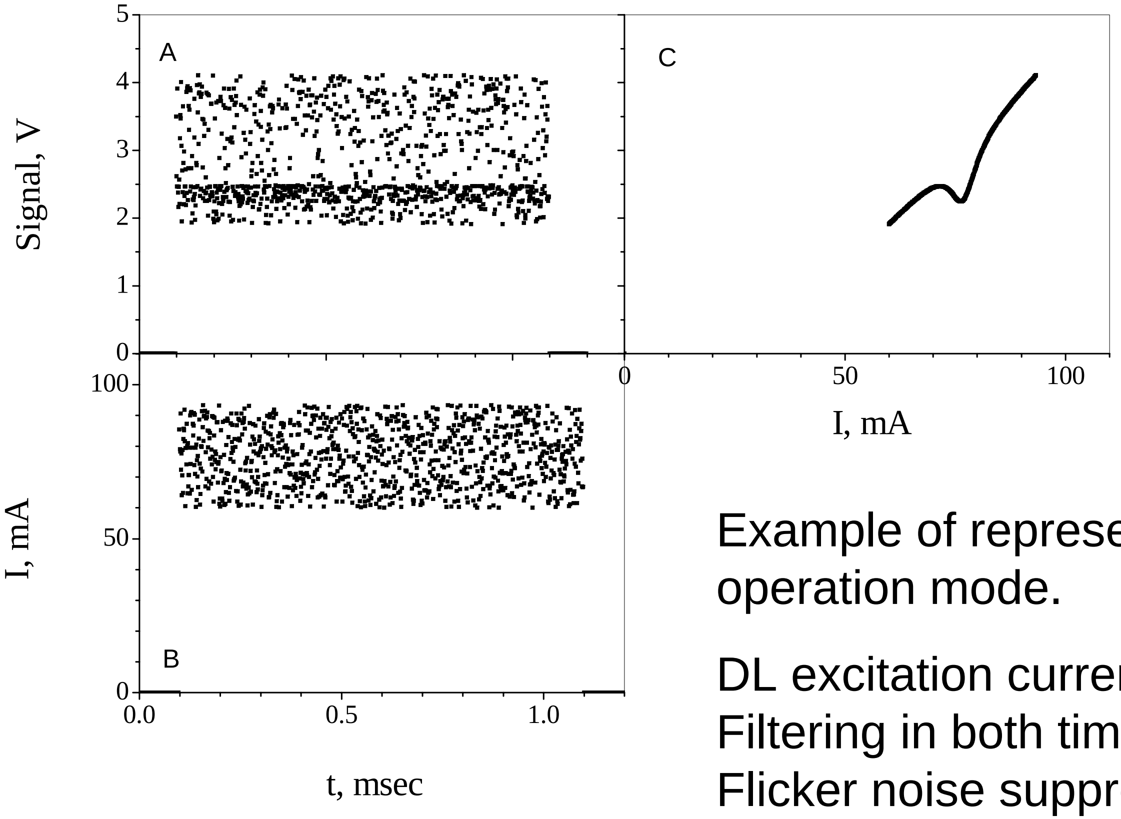
Absorption sensitivity, minimum detectable absorption, noise equivalent absorption.

Comparison of the best known to author results achieved.

For optimized photo-detector system, electronics, and optics usage of generation #3 of TDLS operation mode enable one to achieve fundamental limit of TDLS sensitivity (diode laser quantum noise).

Generation #4

Generation #4 of TDLS operation mode is now in development. It is based on generation #3 technical possibilities, understanding of TDLS physics, and novel technologies.



Example of representative of generation #4 TDLS operation mode.

DL excitation current white noise modulation:
Filtering in both time and frequency domains;
Flicker noise suppression;
Baseline subtraction.