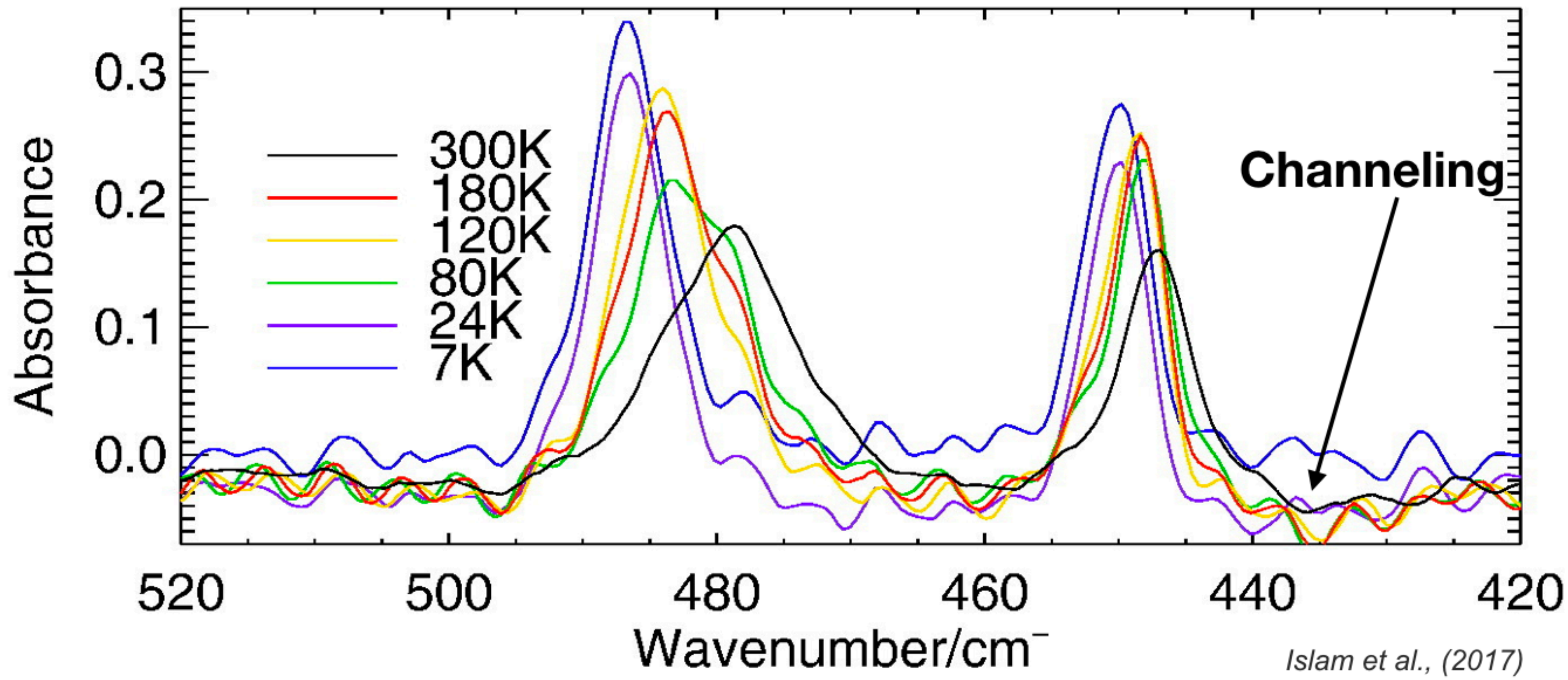
Channeling of the spectra fitted in the SFIT4 code

Channel spectra arise as periodic interference patterns particularly due to reflections in the light path (apertures & filters)



Two models in SFIT4 to fit channeling

The beam correction is applied to the original transmittance t in a microwindow. It creates a zshift-like parameter (z_b) for the Interferogram Perturbation (IP) model, or a complex curvature like scaling factor $\beta_b e^{i\theta_b}$ for the Phase-Shifted reflecting (PS) model:

Background Transmittance_cal zshift

$$y_c = \beta(\Re(T) + z_b + z_0) \qquad \text{IP}$$

$$y_c = \beta(\Re(\beta_b e^{i\theta_b} T) + z_0) \qquad \text{PS}$$

The implementation in SFIT4 takes the following inputs:

- band.*.beam= 0 or number of beams to fit
- band.*.beam.model=PS (phase shifted) or IP (interferogram perturbation)
- band.*.beam.*.apriori=A T φ τ

with A=amplitude, T =period, φ=phase and τ =slope for the amplitude.

The correction to the zshift (z0) is calculated from ζ: let

$$\boldsymbol{\zeta} = A(1+\tau(\mathbf{x}-x_0))\,e^{i\left(\frac{2\pi}{T}(\mathbf{x}-\varphi)\right)}, \text{ then}$$

$$z_b = \Re(\zeta) \qquad \text{IP}$$

$$\beta_b e^{i\theta_b} = 1 - |\zeta| + \zeta \qquad \text{PS}$$

The maximum beam number in SFIT4 = 20

Two models in SFIT4 to fit channeling

$$Y(\nu) = B(\nu) * (Re(T(\nu) * F(c)) + z(\nu)) \quad (1)$$

where $Y(\nu)$ is the calculated transmittance at frequency ν,$B(\nu)$ is the background value at ν,$T(\nu)$ is the complex transmittance at ν after appling apodization and phase error to the interferogram by inverse FFT, with the interferogram produced by using forward FFT to the calculated monochromatic transmittance,$z(\nu)$ is the zero level shift at frequency ν(actually it depends on the bandpass) , and $f(c)$ is a function of the channel parameters c , the expression is given by the following formula

$$f(c) = \sqrt{r_1^2 + r_2^2}\, e^{i\theta}$$

where

$$r_1 = \sum_{j=1}^{NB}\{-c(i,j,1)[1 + c(i,j,4)(v - v_0)] + cos[\frac{A * (v - c(i,j,3))}{c(i,j,2)}]\} \quad (2)$$

$$r_2 = \sum_{j=1}^{NB}\{c(i,j,1)[1 + c(i,j,4)(v - v_0)] * sin[\frac{A * (v - c(i,j,3))}{c(i,j,2)}]\} \quad (3)$$

$A = 6.2831853, v_0$ is the start frequency point of the bandpass interval. NB is the total number of beams in the bandpass i , and apparently r_1 and r_2 are dependent on bandpass, and

$$\theta = tan^{-1}(\frac{r_2}{r_1})$$

(b) Interferogram perturbation model(IP) In this model, channel parameters are fit into the calculation of transmittance by the following expression

$$Y(\nu) = B(\nu) * (Re(T(\nu)) + z(\nu) + p(\nu)) \quad (4)$$

where $p(\nu)$ is defined by

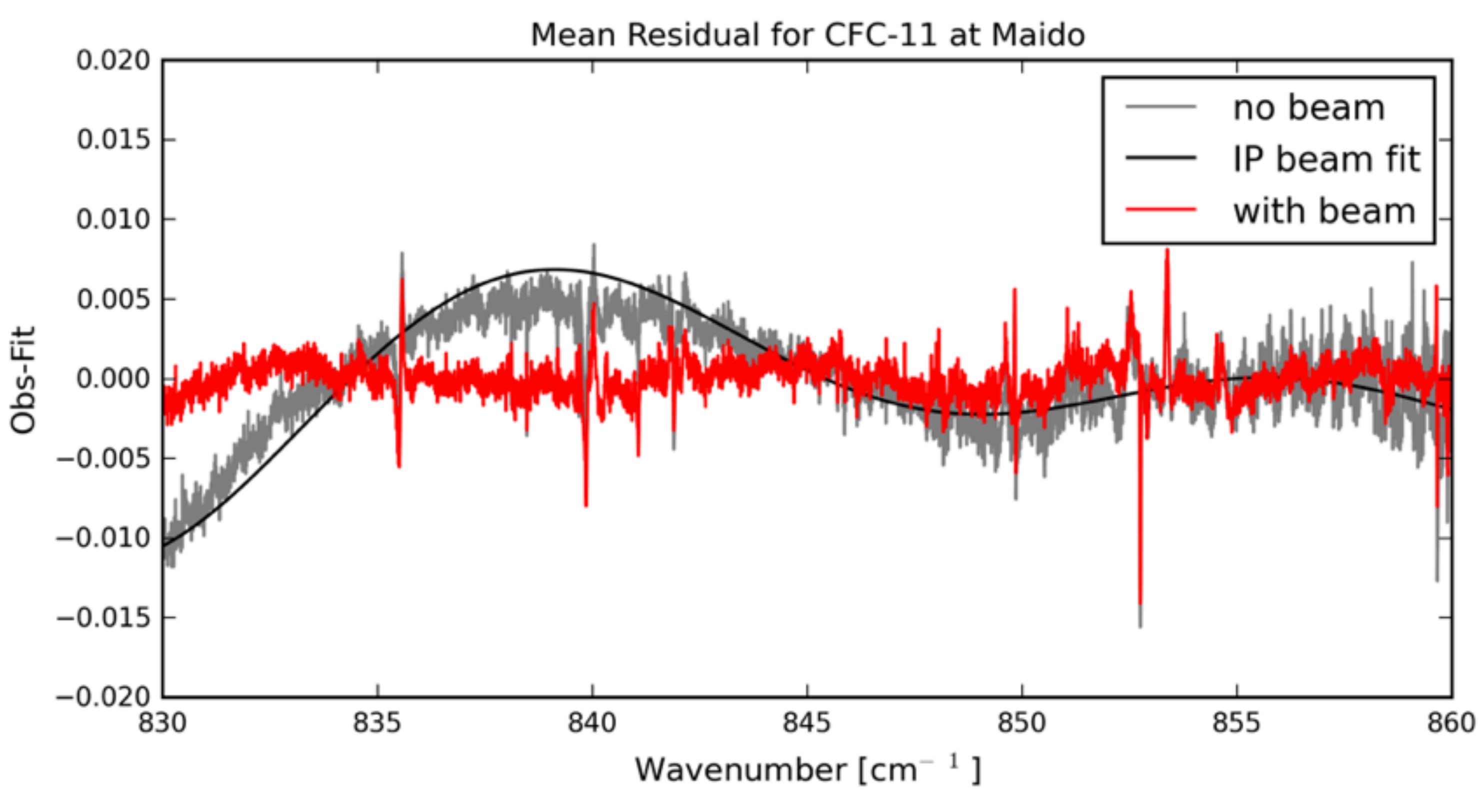
$$p(\nu) = \sum_{j=1}^{NB}\{c(i,j,1)[1 + c(i,j,4)(v - v_0)] * cos[\frac{A * (v - c(i,j,3))}{c(i,j,2)}]\}$$

and $Y(\nu), B(\nu), T(\nu), Z(\nu), v_0$, and NB are the same as in PS mode.

(Wujian Peng 2016)

Discussions

- **Two options (PS or IP) are provided in SFIT4 to handle the channeling, which one we need to choose?**
- **In Vigouroux et al., 2018 HCHO paper, all the PROFFIT sites have a large (7-17%) uncertainty in the channeling, while there is no error budget in the channeling for the SFIT sites**
- **Can we use the beam to fit the background, although it may not due to the channeling spectra? (to some degree, the beam fitting is a tool similar to the slope and curvature to fit the background)**



Discussions

- **If we want to add the error budget from the channeling, how to do it?**

What they do in PROFFIT:
For the channeling amplitude was set to 0.5 ‰
Frequency (0.005), 0.2, 1.0, 3.0 cm^{-1}
50% random/ 50% systematic

Based on the study from Thomas, we know the frequency and amplitude of the channeling at several sites.

Conclusions

- F3: Ampl. is 0.1 to 2.0 ‰, mean: (0.68 +/- 0.48) ‰, median 0.60‰!
- For the paper channeling ampl. was set to 0.5 ‰ in total: Freq.: (0.005), 0.2, 1.0, 3.0 cm^{-1}; 50% random/ 50% systematic
- (Revised) PROFFIT error estimate is quite realistic
- Channeling is not negligible for HCHO error estimate!
- But large scatter: At some places the ampltude is 4 times the mean!
- F6: Ampl. is 0.3 to 21 ‰, mean: (2.45 +/- 4.50) ‰, median 1.2‰!
- Even larger as compared to InSb filter 3!
- Channeling is not negligible!
- Needs to be reduced at many sites before analysing weak signatures, e.g. of $ClONO_2$, SF_6 …!
- Channeling mostly due to B/S, in part. due to the wedge of the gap!
- In contact with Axel Keens to improve this in the future.

Thomas Blumenstock May, 2019