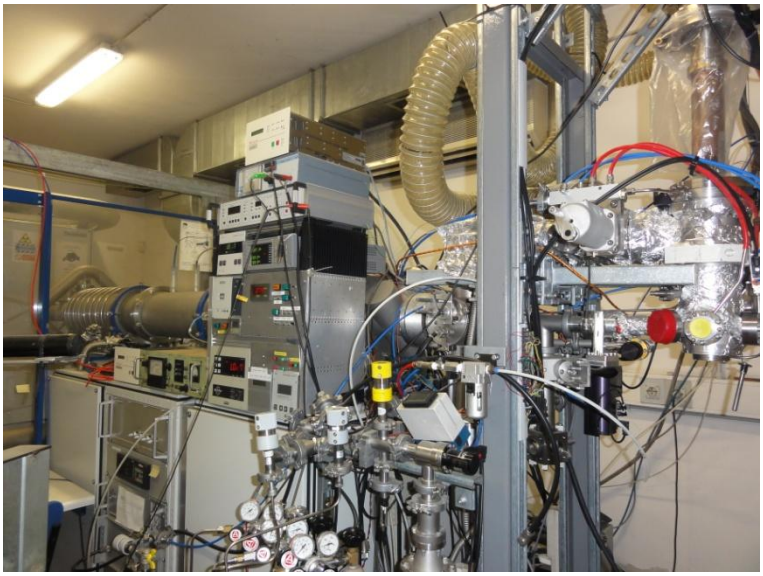
Guide for the tool "ICE Thickness Calculator"



LASp: Laboratory for Experimental Astrophysics

Osservatorio Astrofisico di Catania

C.SCIRE'[1]

(1) INAF – Osservatorio Astrofisico di Catania

Technical internal report

N. 1/2017

1. Overview

A laser beam directed towards a system composed by a thin film of ice deposited on a substrate, gives reflections at the interfaces vacuum-film and film-substrate. For a thin optical film interference is observed and constructive and destructive superposition of the reflected beams form a characteristic interference pattern during the deposition of the ice that can provide film thickness information.

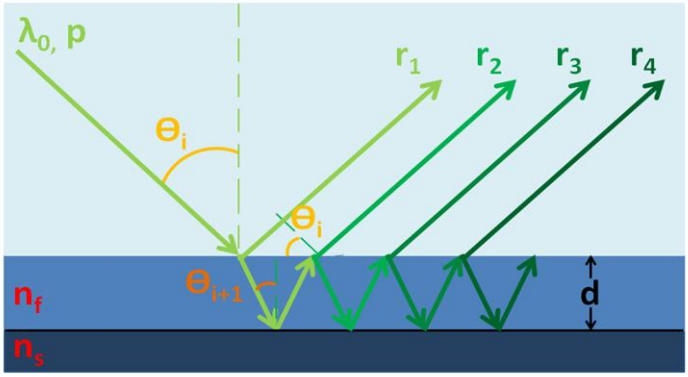
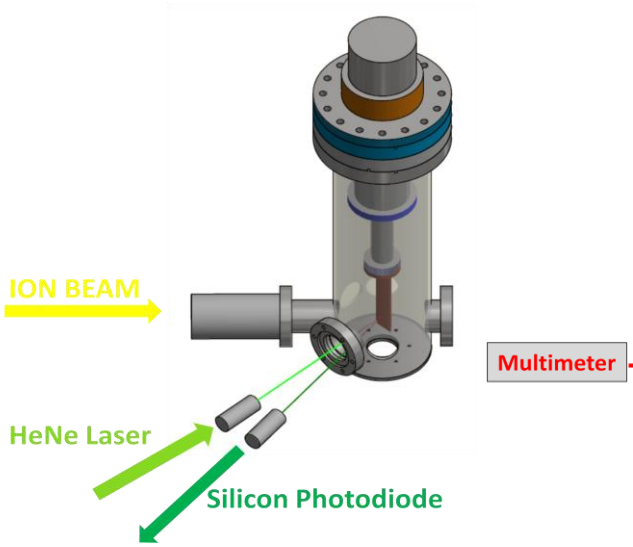


Fig.1 System medium-film-substrate

In our experimental set up, a He-Ne laser is used to monitor the ice thickness during the deposition by allowing us to look at the interference pattern given by the laser beam directed toward the sample and reflected at few degrees both by the vacuum-ice and ice-substrate interfaces. The reflected laser beam is then detected by an external silicon-photodiode detector, analyzed by a multimeter and recorded by a computer routine.



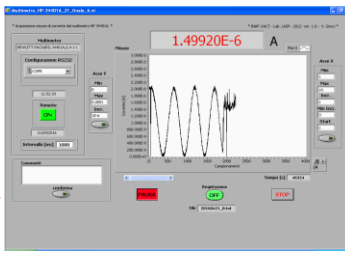


Fig.2 Actual Experimental Set-Up

Fig.3 Computer Processing

2. Work Purpose

The aim of this document is the description of a tool called "*Ice Thickness Calculator*" that can be used for the thickness calculation of a thin ice film deposited on a substrate.
The program is based on the laser interference technique in which a laser beam is directed toward a film and the superposition of the reflected light produce an interference curve during the film accretion.
The tool is available at the web address: http://www.oact.inaf.it/thickness/
Basically the input data can be written in the web main interface and are read by the program 'SPESS' (written in FORTRAN language) that, by using a numerical method [1], will compute the output refractive index and the period of the interference curve (given in thickness units) that are shown in the results web page.
The user has also the possibility to download the theoretical interference curve, calculated by the program in ASCII format, that can be used to compute the film thickness, with a good accuracy, at an arbitrary point of the experimental interference curve acquired during deposition (see section 5).

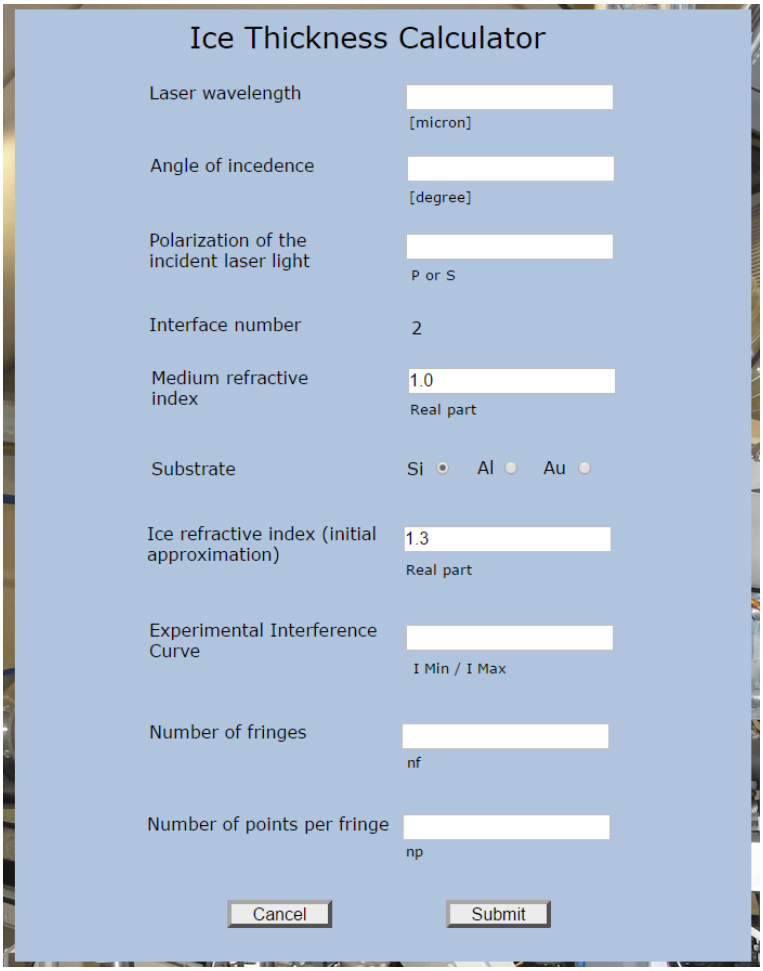


Fig.4 Main web interface

3. The SPESS program

In general the reflectance (R) of a thin film deposited on a substrate can be represented by a function of: the laser wavelength (λ_0), the refractive index of the film (n_f), the refractive index of the substrate (n_s), the film thickness (d), the incident angle (Θ_i with respect to the normal) and the polarization of the laser light (p):

$$R=f(\lambda_0, n_f, n_s, d, \Theta_i, p) \qquad (1)$$

At a fixed wavelength, if we assume that there is no absorption in the film at the laser wavelength, R is a periodic function of the thickness and the period, that is the distance between two maxima or two minima in the interference curve (reflectance R versus the film thickness), is given by the equation:

$$\Delta d = \frac{\lambda_0}{2n_f\sqrt{1-sin^2\,\Theta_i/n_f^2}} \qquad (2)$$

From eq. (2) it is evident that n_f, the refractive index of the film, must be known in order to measure its thickness. The amplitude of the interference curve itself depends on the refractive index of the sample, so by measuring this quantity (intensity ratio between maxima and minima) it is possible to derive the refractive index of the ice and then the thickness.
In eq. (1) λ_0, n_s, Θ_i and p are known quantities, so for a given refractive index of the film we can compute an interference curve (R versus the thickness d). We derive the refractive index of the film by using a FORTRAN code, named SPESS, that varies the n_f value until the theoretical amplitude of the interference curve becomes equal to the experimental one.

4. Interface

The web interface has a multi-user arrangement. Once the input data are written in the input form, the interface create a file named SPESS***.INP (where *** is a progressive number assigned to each work session) containing the input data; the file is then read by the SPESS FORTRAN program that calculate the best fit solution for the film refractive index which better reproduces the experimental interference curve amplitude.
The results are written in a file and are shown in the results page of the web user interface.
The interface was designed to be user-friendly: comments are provided to help the users to fill in correctly the form fields.
In general the computation take place under some specific conditions (fixed input parameters), in particular: there are only two interfaces (vacuum-film and film-substrate) and the considered substrates are completely opaque at the laser wavelength (the reflected light at the second substrate interface can be neglected).
Furthermore some defaults value are preset.

The form has the following input fields:

Laser wavelength
The optimal laser wavelength depends on the chosen substrate, this value can be varied between 0.2 and 10 micrometer.

Angle of incidence
The angle of incidence of the laser with respect to the normal of the ice surface, the value can be varied between 0° and 90°.

Polarization of the incident laser light
The laser polarization can be of P type (if the electric vector of the incident electromagnetic radiation is parallel to the plane of incidence) or S type (if the electric vector of the incident electromagnetic radiation is perpendicular to the plane of incidence).

Interface number
The interfaces are two, one between the medium and the film and one between the film and the substrate.

Medium refractive index
The refractive index of the medium, the default value is 1.0 suitable for a vacuum medium or, in first approximation, air.

Substrate
At the moment it is possible to choice between three of the most common substrate that are completely opaque to the visible light: Silicon, Aluminum and Gold.
Further details for the substrate and laser wavelength choice can be found in [4].

Ice refractive index
In this field the initial approximation for the refractive index of the film has to be inserted, here the default value is 1.3 as water ice.

Experimental Interference curve
Here it has to be inserted the ratio between the first Minimum and the first Maximum of the experimental interference curve in order to consider the curve normalized to 1. In this way it is possible to use the reflectance measurement in linear arbitrary units for the interference curve acquisition.

Number of fringes
Number of fringes of the output theoretical interference curve, the value has to be between 1 and 30.

Number of points per fringe
Number of sample points for each fringe of the output theoretical interference curve, the value has to be between 40 and 400.

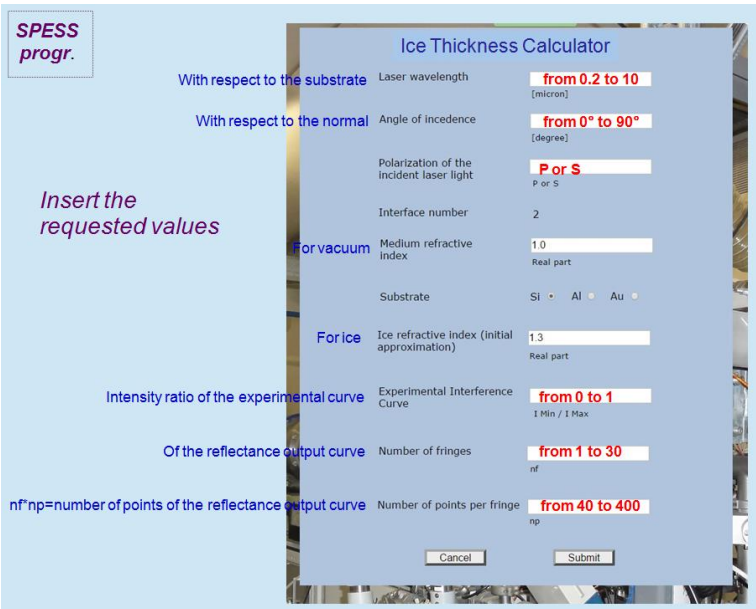


Fig.5 Main web interface with the comments

After the calculation performed by the SPESS program, in the result page the following fields are shown:

Film refractive index
Film refractive index calculated by the program.

Interference curve period
Theoretical interference curve period in micrometer.

Quality factor
Quality factor for the best fit calculation, 1 for the optimal solution.

Substrate refractive index
Substrate refractive index with respect to the used laser wavelength.

Download the interference curve
Download button for the theoretical interference curve file in ASCII format.

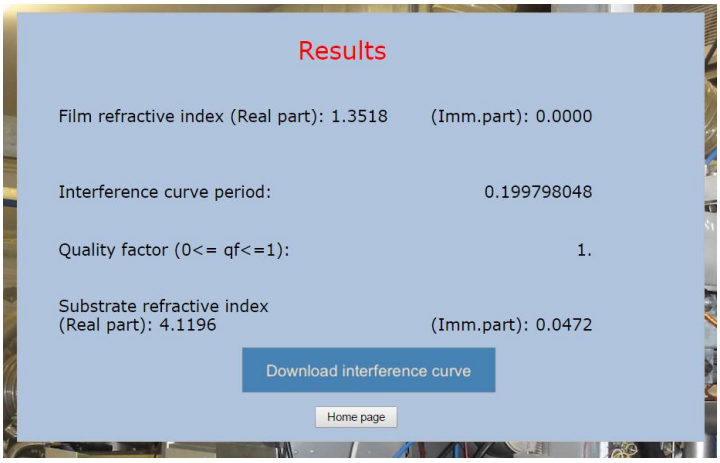


Fig.6 Results web page

5. Measurement method

Following the theoretical interference curve, as calculated from the program and normalized:

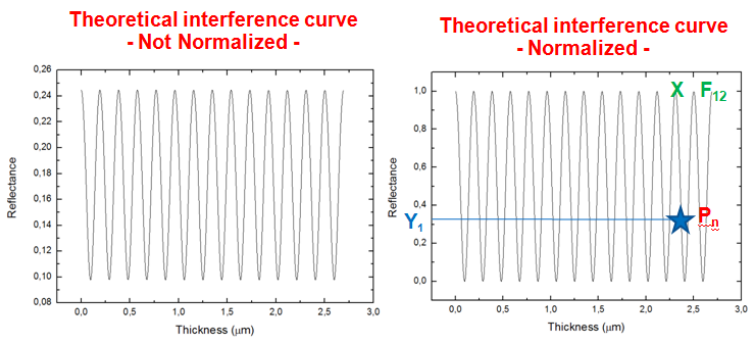


Fig.7 Theoretical Interference Curve

From the comparison between the theoretical interference curve and the experimental one, both normalized from 0 to 1, it is possible to derive with a good accuracy the film thickness:

1) A given point (P_n) in the experimental normalized interference curve is identified on the theoretical interference curve at the given normalized ordinate (Y_1) and at the given fringe number (F_{12}).
2) The corresponding abscissa found in the normalized theoretical interference curve represents the thickness.

Instead of normalizing the full experimental interference curve it is possible to obtain the normalized intensity of the P point by using the formula:

$$Y_1 = \frac{(Y_0 - Y_{MIN1})}{(Y_{MAX1} - Y_{MIN1})}$$

where MIN1 and MAX1 are the closest minimum and maximum to the point.

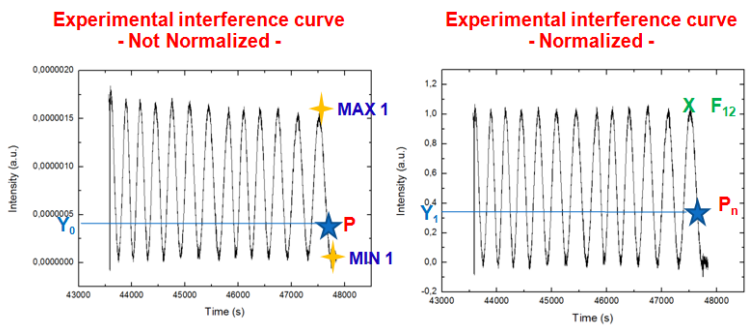


Fig.8 Experimental Interference Curve

The absolute accuracy of this measuring method is approximately equal to 5%.
The precision of the calculation is affected by the uncertainty in the knowledge of the optical constants of the substrate at low temperature and the measuring error of the laser incidence angle.
Further details for the thickness measurement method can be found in [1], [2], [3], [4].

References

[1] G.A. Baratta & M.E. Palumbo, *Infrared optical constants of CO and CO_2 thin icy films*, J. Opt. Soc. Am. A/ Vol. 15, No. 12/December 1998.

[2] D. Fulvio, B. Sivaraman, G.A. Baratta, M.E. Palumbo, N.J. Mason, *Novel measurements of refractive index, density and mid-infrared integrated band strengths for solid O_2, N_2O and NO_2:N_2O_4 mixtures*, Spectrochimica Acta Part A 72 (2009) 1007–1013.

[3] P. Modica & M.E. Palumbo, *Formation of methyl formate after cosmic ion irradiation of icy grain mantles*, A&A 519, A22 (2010).

[4] R. G. Urso, C. Scirè, G. A. Baratta, G. Compagnini, and M. E. Palumbo, *Combined infrared and Raman study of solid CO*, A&A 594, A80 (2016).