User Manual

This document describes the functionality of the *Thermal Evaporation Simulator*.
Thermal evaporation is a method used to produce thin films. Targets play an important role in nuclear physics experiments, and a proper knowledge of their thickness is crucial. With this GUI we model the evaporator of the Target Design Laboratory (TDL) of LIP (located in FCUL) and the main goal of this project is to give a good estimation for the thickness of the film.
Inside the evaporator you can see the source holder called “boat”. There are many different types of boats. Above the boat it is the substrate where the source particles will be deposited.

The process of thermal evaporation is based on the Hertz-Knudsen equation, where P_{vp} is the vapor pressure of the source, P_{amb} is the pressure inside the evaporator, *M* is the molar mass of the source, *T* is the temperature to which the source is subjected:

$$\phi = \frac{\alpha N_A (P_{vp} - P_{amb})}{\sqrt{2\pi MRT}}$$

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Assumed Conditions

Evaporated Mass

We will consider all the mass evaporated.

Chamber's Pressure

The pressure inside the chamber of evaporation (or chamber pressure) is considered constant.

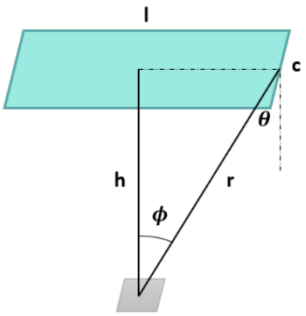
Source Temperature

The temperature of the evaporation source is considered to be constant and the minimum required for thermal evaporation to occur.

Geometry

Given the geometry of this problem the thickness along the substrate is described by spherical coordinates:

$$t = \frac{M_{evap}(n+1)cos^{n}\phi cos\theta}{2\pi r^{2}}$$



There are three possibilities of particle distribution that the user can choose (based on the boat, for example): ideal isotropic (n=0), ideal anisotropic (n=1) and truncated isotropic.
For more information regarding how each initial condition is defined, please check the sub-section "Required Inputs".

User Interface

As our evaporator doesn't have a quartz balance it is important to be able to predict the thickness along the surface of the substrate. The user interface is where you are able to interact with the program to simulate the thermal deposition process and have an estimation of the films' thickness and uniformity, as well as the minimum temperature required to evaporate the source at a given pressure. For that, some tools are provided to better help with such tasks.

Here is a brief overview of the general aspects of the user interface. At the left top corner of the GUI's window, there is a toolbar. As the eyes start to wander around the window, you will see the drop-down menus, entry/input boxes and buttons where you select, type and click according to what you want to do. On the right, you see a graph with geometric figures - this is a 3D display of the simulation's setup you are generating.

The Interface's Toolbar

The GUI's Toolbar is an easy way to access the different tools the program offers. There are three buttons: 'Home', 'Database' and 'Manual'.

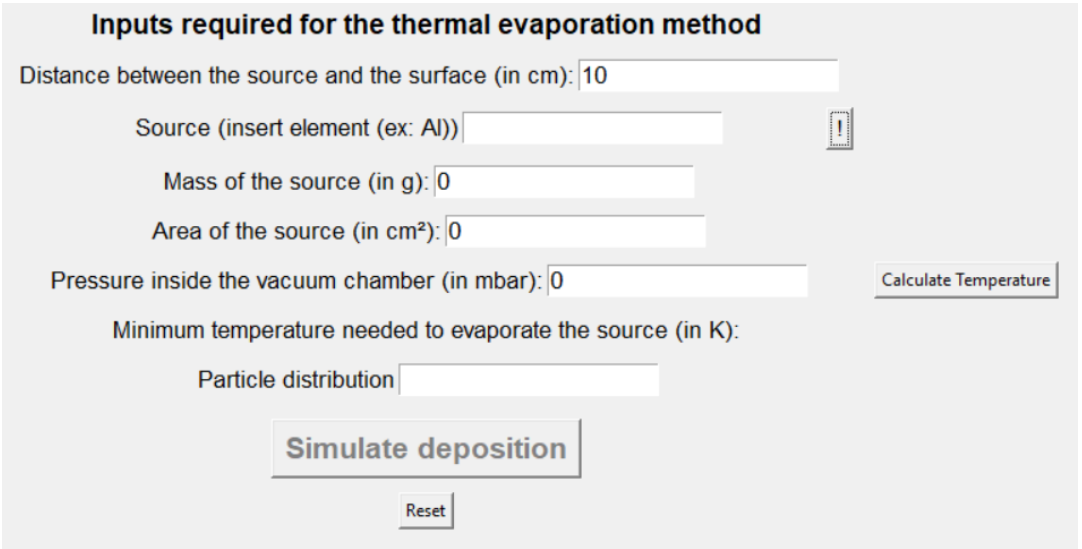
- 'Home' - Upon clicking this button, two options will be displayed: 'Reset' and 'Exit'. The 'Reset' button will close the current window and open a new one, while the 'Exit' button will simply close the window.
- 'Database' - This button opens a new window when pressed, which showcases the database created for this project. In it, you may find all the possible materials to choose for your evaporation source and their characteristics.
- 'Manual' - This button opens a new window with the User Manual, which you are now reading.

Required Inputs

As our evaporator doesn't have a quartz balance it is important to be able to predict the thickness along the surface of the substrate. This tool requires from the user some obligatory inputs for the thermal evaporation process to be simulated.

1. Distance between the source and the substrate;
2. Material to evaporate;
3. Mass of the source;
4. Area of the source;
5. Distance between the source and the substrate;
6. Pressure inside the evaporator;
7. Evaporation distribution.

Below, there is a showcase of where the user should insert such inputs in the GUI, with the numbers corresponding to the previous enumerated list.



Buttons' functionality

From the previous figure, you can see four buttons. Each one has a different function.

‘!’ - warning: the user can only choose elements that are presented in our database.

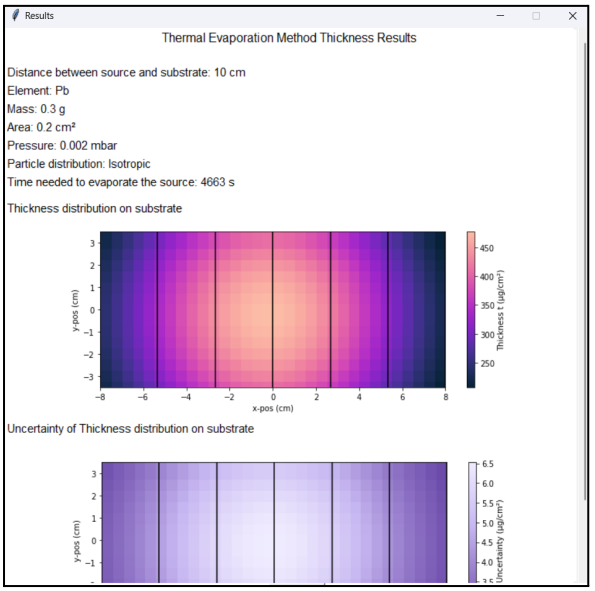
‘Calculate Temperature’ gives the minimum temperature needed to evaporate the specified source for the defined chamber pressure. For that, the program solves the extended Antoine equation for the temperature. The equation has the following expression:

$$log(P/atm) = A + BT^{-1} + C\,log(T) + DT^{-3}$$

The values of A, B, C and D for any chosen material can be searched for in our database.

‘Simulate deposition’, as the name implies, starts the simulation of the thermal deposition process. A window is automatically opened displaying graphs, one with the film’s thickness along the substrate and the other with the corresponding uncertainty, but also displaying the initial conditions/inputs the user has given. For more information on this last part, please check the previous sub-section.

Below, you can see an example of the display window.



You can see all the information using the scrollbar on the right side.

‘Reset’ has the only purpose to clear all the input boxes and values, as well as reset any simulation or temperature output that the GUI has previously given.

Package Usage

This program was implemented in Python 3.8.5 and tested in Jupyter Notebook 6.1.4. So, before running the program, please be sure to have installed the correct Python version; also, be sure to have the following packages/modules from Python on your machine for the correct functioning of this program:

- *tkinter*
- *numpy*
- *matplotlib.pyplot*
- *math*
- *openpyxl*
- *scipy.optimize*
- *sympy*
- *BytesIO from io*

- *pandas*
- *random*
- *PIL*

Tkinter

The tkinter package (“Tk interface”) is the standard Python interface to the Tcl/Tk GUI toolkit.

NumPy

NumPy is a Python library that provides a multidimensional array object, various derived objects (such as masked arrays and matrices), and an assortment of routines for fast operations on arrays.

Matplolib.pyplot

Matplotlib graphs data on Figures (e.g., windows, Jupyter widgets, etc.), each of which can contain one or more axes, an area where points can be specified in terms of x-y coordinates.

Math

Module containing various mathematical functions in Python.

Openpyxl

Python library that allows the handling of Excel spreadsheet files.

Scipy.optimize

Provides tools for solving mathematical optimization problems.

Sympy

Sympy is a Python library for symbolic mathematics, enabling symbolic computation, algebraic manipulation, calculus, equation solving, and more.

io

The 'io' module offers tools for handling various types of I/O (input/output) operations in Python.

Pandas

Primarily used for data manipulation and analysis.

Random

The 'random' module provides functionalities for generating random numbers, sequences, and performing random selections and operations in Python.

FAQs and troubleshooting

- Tkinter window size affected

If you run the GUI in Visual Studio Code or Python and you click on the ‘Simulate deposition’ button the window will change size and the process behavior of the individual frames will not

look the same. Unfortunately, we are not sure why this happens and if it happens on any computer or operating system. We advise you to run this simulation in Jupyter Notebook, as this issue was not observed.

- Can I save the results?

Yes, once the window with the results opens you can see an option saying ‘Save as pdf’. After that you can choose the name of the file and the folder.

- Can I save the individual plots displayed on the window results?

Yes, upon running the simulation, the plots are promptly saved within the directory where your code resides. However, if you click on the reset button they will be erased. Change the names of the figures if you don’t want that to happen.

Last modified: 8 january 2024

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