pyDAMPF: A Python Package For Modeling Mechanical Properties Of Hygroscopic Materials Under Interaction With A Nanoprobe

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INTRODUCTION

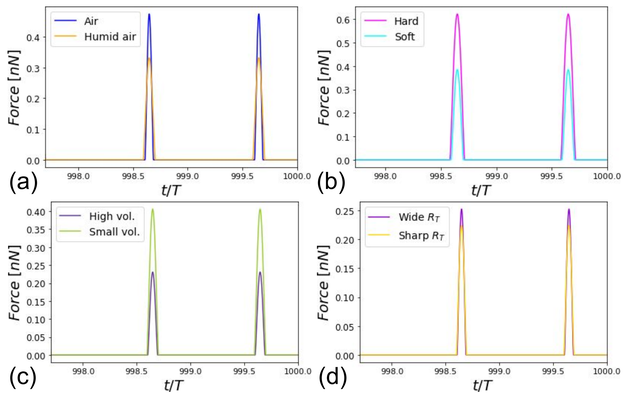
pyDAMPF is a tool oriented to the Atomic Force Microscopy (AFM) community, which allows the simulation of the physical properties of materials under variable relative humidity.

The current project has 3 goals:

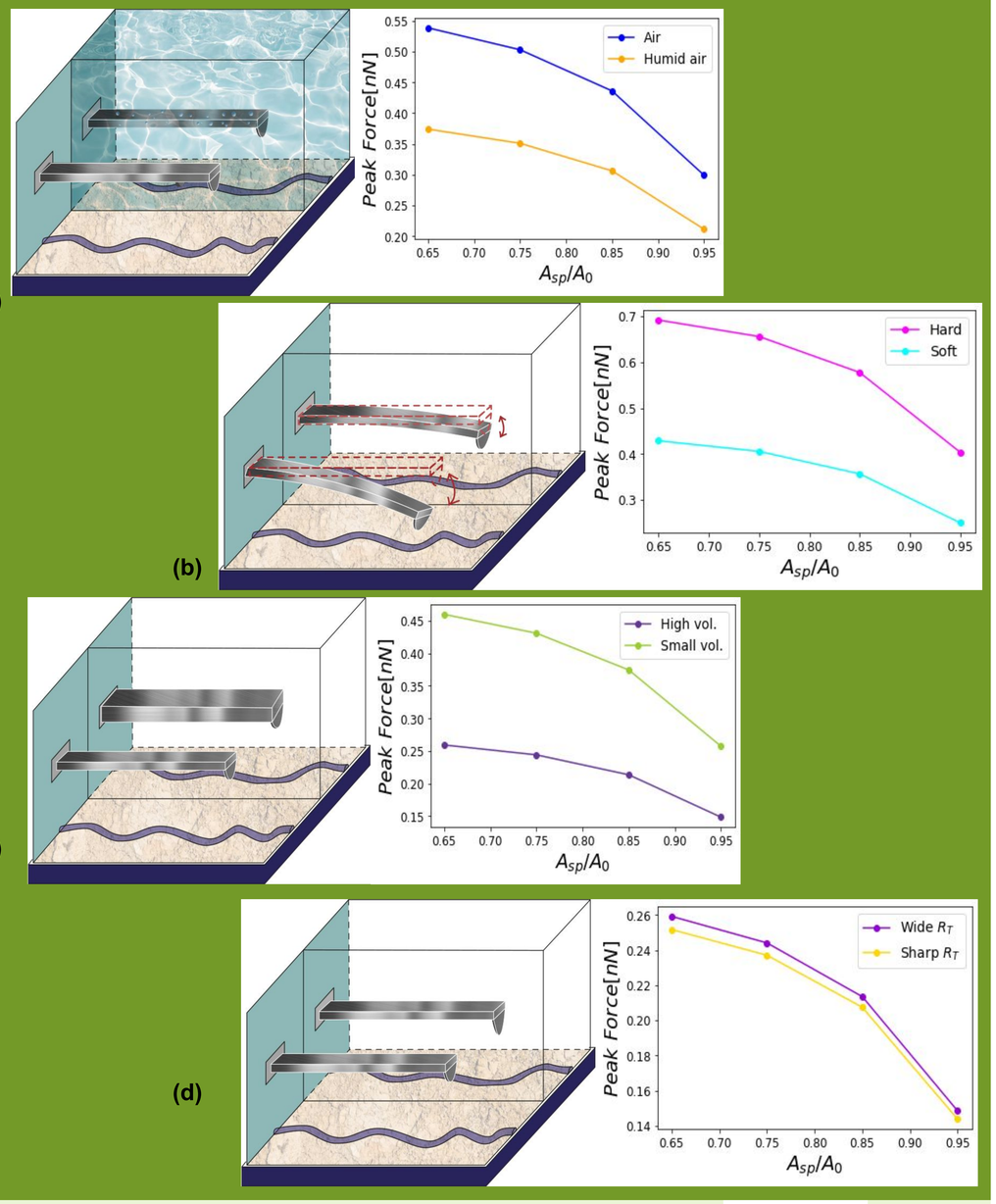
1. Modeling the mechanical properties of hygroscopic nanofibers with the pyDAMPF package.
2. Present four scenarios comparing different microscope probes (AFM cantilevers) and the same sample, namely PolyVinyl Acetate (PVA) fiber.
3. Implement a highly time-efficient execution method to deliver results at least an order of magnitude faster than existing approaches.

METHOD

pyDAMPF software has been developed with a variety of models for deeper analysis of mechanical properties at the nanoscale, with a numerical core in Fortran wrapped in Python, with a self-developed parallel execution method, to achieve greater efficiency in execution times. For more details please scan the QR code.



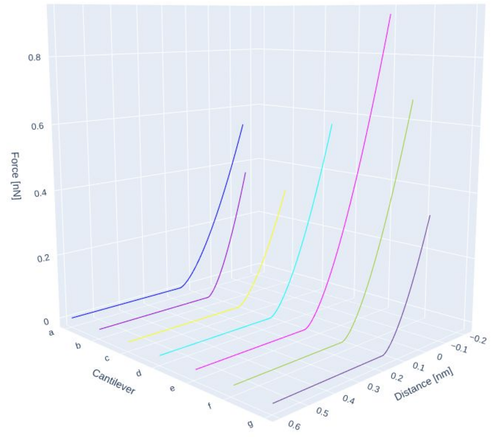
IT'S AMAZING WHAT YOU CAN DO WITH AN IN-HOUSE CODE!!!



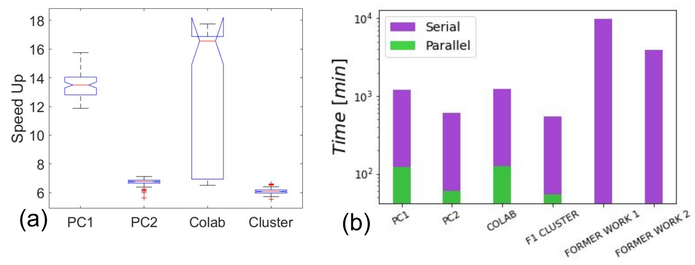
pyDAMPF

RESULTS

pyDAMPF is capable of displaying various figures of interest, we show a figure in which the user can see the force vs. distance curves and compare the different AFM probes.



Comparing execution times.



DISCUSSION

- pyDAMPF is a highly efficient and adaptable simulation tool aimed at analyzing, planning and interpreting dynamic AFM experiments.
- Easy to use for scientists without a computing background, in particular in the use of multi-threads.
- It supports the addition of further AFM cantilevers and parameters into the code database.
- Allows an interactive analysis, including a graphical and table-based comparison of results through Jupyter Notebooks.