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Bio-inspired Omniphobic Surfaces (BIOS): Process development for producing at scale omniphobic and drag free plastic surfaces

15 April 2021

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1. Research Summary

The main objective of this project is the development and application of an accurate model for the prediction of wetting behavior. Wettability was identified as the most prevalent mechanism associated with adhesion of liquids onto their enclosing material [1]. The overarching goal is to assist in the design of surfaces, e.g., of packaging materials or storage units, that repel the enclosed liquids as much as possible. This leads to saving a substantial amount of consumable commodities (e.g., water) and other domestic products (edible or not) of daily life. Besides saving food, controlling surface wettability has a great impact in other technological domains investigating, for example, non-wetting textiles [2, 3], anti-fogging/icing windowpanes [4, 5] and car windshields, improved hydrodynamics [6], buoyancy [7] and water collection from fog [8].

Existing state-of-the art models suffer from low accuracy [9, 10], while they are subject to rather oversimplifying assumptions which hold true only in certain special cases. In this project, we developed an accurate model for the prediction of surface topographies that exhibit omniphobicity, i.e., strongly repel all sorts of liquids [11]. This was accomplished by considering realistic curved liquid-air interfaces with the help of the sagging height which, in turn, was defined through the capillary length [12]. Single, double and triple level topographies were integrated into the predictive algorithm, while different combinations of the two were made possible. Our model showed that multiscale hierarchical roughness is a promising way for achieving enhanced liquid repellency [11, 13, 14].

In our latest work, we reported the development and application of a refined version of the classical Cassie-Baxter wetting model [15] for the prediction of surface topographies with superomniphobic traits. The sagging height defined through the capillary length was utilized to assess the relation between a curved liquid-air interface and the surface texture. The wettability, expressed in terms of the static apparent contact angle, was quantified for single- and double-scale surface topographies and for three representative liquids and the results were compared to those of the classical Cassie-Baxter model. Of the three single-scale topographies considered in this work, the fiber case exhibited the highest contact angle across length scales of surface topographies, whereas decreasing the length scale of surface patterns from a few hundreds of micrometers to a few hundreds of nanometers led to contact angle increase by

15%–20%.A generic expression for modeling multiscale hierarchical roughness of arbitrarily large multiplicity n was derived and applied. Multiscale hierarchical roughness was corroborated to be a promising way for achieving enhanced liquid repellency. Double-scale roughness was more efficient when the two length scales differed in size by at least one order of magnitude. The 'fiber on sinusoid' hierarchical topography exhibiting re-entrant geometry yielded contact angles over 150° for all considered wetting liquids. Our model predictions were very recently validated against experimental data for a broad variety of surface materials, topography types, hierarchical levels and dimensions.

2. Description of the data

The generated data is divided into six different **types** (see below for details):

2.1) Source code: the executable of the compiled and built source code that performs the calculation, as well as the source code itself.

2.2) The required input files in order to define the specifics of the calculation (material type, material properties, topography type, variable ranges, etc.)

2.3) The generated output files containing the calculation results.

2.4) Post-processing scripts for the visualization of the generated results.

2.5) Metadata: Documentation files are provided for all the above types of data containing instructions on how one can proceed in order to i) understand the code capabilities, ii) fill in the required input files, iii) run the calculation, iv) generate and collect the output data and v) post-process the obtained results with a graphical analysis tool for visualization and assessment

2.6) An "Example" directory containing an indicative set of results in the form of raw data, as well as processed results with the help of the visualization tool (see d) in the form of figures, graphs, tables etc.

The **format** of the data is again divided into the following categories depending on the **type** of data according to the categorization scheme given above:

a) For the source code: the source code is given in the form of a precompiled and built executable binary file that may run on any Linux/Unix machine following the detailed instructions provided in the detailed documentation alongside the executable. Instructions on how to create an executable for Windows are provided alongside the source code.

b) The required input files are simple ASCII text files that can be read and edited by any text editor.
c) The generated output files are also simple ASCII files that can be imported and processed seamlessly and effortlessly into any visualization, plotting or data analysis software.
d) The post-processing tool is an ASCII file enclosing a script suitable to run in the Gnuplot graphing utility.
e) The metadata files constitute documentation files having the format of common text files (e.g. docx or csv)

The **volume** of four of the above data types (source code, input file, plotting scrip and the documentation) is, at the most, on the order of a few megabytes. The volume of the "example" directory is on the order of a few tens of megabytes for the selected example case, while, the volume of the output files varies anywhere between a few tens of megabytes, for the simplest cases considered, to a few gigabytes for the most detailed calculations, depending on the specifics of the modelled cases. The produced data, in its entirety, is free to be used and disseminated and is not bound to any kind of IP restrictions. However, any type of usage of the generated data and/or metadata should always be accompanied by reference to the original publication (doi.org/10.1088/2051-672X/ab9419).

The uploaded data is divided into the following categories (directories):

Short code description:

This code calculates the contact angle formed between a sessile drop of an arbitrarily defined liquid and a rough surface based on our improved Cassie-Baxter wetting model (https://doi.org/10.1088/2051-672X/ab9419). The topography of the surface needs to be predefined into the input file and may be any of the types: a) 2D pillars, b) fibers, c) sinusoids, d) 3D pillars. The code may model up to three-level topographies hierarchically placed on top of one another. In the "Input" directory, three input files are given for single, two-level and three-level topographies, respectively. In multilevel topographies, the above-mentioned topography types may be combined at will. So, for example, we may have a three-level topography with sinusoidal pulses as the coarser level, fibers as the middle-level and 2D pillars as the finest level. Similarly, two-level and single-level topographies are also possible. The definitions of the multiplicity level and topography types proceed in the input file.

2.1) Executables to run the code:

Depending on what kind of environment you are using, we have included one executable file in the “1_executables_&_SourceCode” directory, for Linux machines. For Windows users, we have included the Source Code along with instructions (see 5_Instructions directory) on how to build a Windows-compatible executable and how to run it. Regardless of the operating system, you need to make sure that the executable and the input file named “input.in” are in the same directory. If you are on a Linux machine, open up a terminal and navigate to the directory where the executable “run_linux” is and then simply type “./run_linux” and the code will run. If you are on a Windows machine, navigate to the working directory where the executable is by using a file explorer and simply double click on the executable “run_windows”.

2.2) Input file:

The input file contains necessary information on the wetting liquid, surface material, topography type and multiplicity and characteristic dimensions for each topography level. Example input files for single-, two- and three-level topographies are included in the “2_input_files” folder. These input files can be opened and edited by any text editor. Input is read by the code line-by-line, while comments are included in each line of the input file.

In the first line of the input file, the total, polar and dispersive components of the surface tension of the wetting liquid in [N/m] are required. In the example input files, water is considered to be the wetting liquid. The polar and dispersive components are not necessary to be known, however a value must be given (it may be any value if they are unknown). These values are used in case the Young’s contact angle for that specific set of liquid/surface is unknown, so that it will be estimated by using the Owens-Wendt relation.

In the second line, the liquid density is required in [kg/m^3].

In the third line the total, polar and dispersive components of the surface energy in [N/m] are required. Again, like above, the total and dispersive components do not need to be necessarily known. They are used in the estimation of Young's contact angle in case it is unknown. However, even if not required, a value must be given.

Next, the Young's contact angle formed by the wetting liquid (in the examples water) and a completely flat surface made of the same material as the considered rough surface is required in degrees. After that, the number of topography levels (multiplicity) is given. In the "2_input_files" directory, we have provided example input files for up to three superposing topography levels. The code of course can handle an arbitrarily large multiplicity. In the next line, the name of the output file is given. Below that, the first (coarser) topography type is defined by an index integer number: 1=pillar, 2=fiber, 3=sinusoidal, 4=3Dpillars. After that, a value range of the characteristic lengths of each topography as defined in our publication (https://doi.org/10.1088/2051-672X/ab9419) are given. For example, for the 2D pillar topography, we need to specify parameter l_0 in [m], next the pillar width in [μm] and next the pillar distance in [μm]. The last input is the pillar height in [μm] as a single value (not range) and is applicable only when the pillar topography is selected. If the multiplicity is larger than 1, then below that follows the dimensional information on the second topography level similar to the first, i.e. parameter l0 of the second level, etc..

2.3) Output file:

Once the calculation is complete, one output file is generated. The output file will have the name specified into the input file (see point 2). Depending on the multiplicity of roughness, a different number of columns will be included. For every roughness level, the dimensions of the characteristic lengths are given in equally numbered columns and then the calculated contact angle. Finally, there is a last column containing debugging information. For example, for a sinusoidal single level topography, four columns will be generated: the first one will be the amplitude of the pulse, the second one the wavelength and the third column the calculated contact angle. The last column shows which wetting scenario prevails for this particular set of dimensions. The format of the file is ideal for plotting by using conventional graphical software such as gnuplot or Xmgrace.

2.4) Post-process:

In the simplest case of single-level roughness, a three-column file will be generated which can be easily plotted in a 3D plot (e.g., heat map). For larger roughness multiplicity, the number of columns (corresponding to characteristic length parameters of each roughness level) increases and is difficult to plot. In these cases, the results can be illustrated in a tabulated form. A post-process script for creating a 3D heat map for a single-level sinusoidal roughness is provided in the "4_visualization" directory. The result of such a post-processing can be viewed in the example 3D heat map contained in the "6_Example" directory.

2.5) Documentation:

Detailed instructions on how to set up and run the calculation, as well as suggestion on how to analyze and visualize the results are provided in a separate directory named "5_Instructions".

2.6) Examples:

An example directory, named "6_Example", has been created for demonstration purposes. In that directory, one may find an output file generated after running the code for a single-level sinusoidal topography, as well as an indicative plotting script for creating with Gnuplot a 3D representation (heat map) of the results. An image of such a generated heat map is also included in the same directory.

3. Existing databases and justification

Currently, there is a large multiple of data repositories in the area of Materials Science; characteristic examples include (but are not limited to): the Materials Data Facility (https://fairsharing.org/biodbcore-001780/), NanoCommons Knowledge Base (https://fairsharing.org/biodbcore-001485/), INPTDAT – The Data Platform for Plasma Technology (https://fairsharing.org/FAIRsharing.2VADoR), the NOMAD Laboratory (https://fairsharing.org/FAIRsharing.aq20qn) just to name a few. Representative archives of available data repositories can be found at https://fairsharing.org/biodbcore/ or at https://www.re3data.org/. For someone not sure where to deposit their data, these webpages constitute a nice place to start. Usually, data repositories are divided into categories based on discipline, field or research area. Additional filtering criteria such as, e.g., country, database access, data licenses and data access restrictions may apply as well based on the type and nature of the data.

Data repositories dedicated to Materials Science can be found easily by searching the key word “Materials Science”. As can be seen, the resulting list of data bases is very general; some data bases do not comply with the FAIR principles, some others are accessible at a cost, while some others are specific to a certain subdomain of “Materials Science” such as Plasma Technology, Crystalline materials or Nanomaterials, etc.. A very important aspect in the selection process of a data repository is related to its trustworthiness. This is manifested by the so-called data seal of approval (DSA). The DSA gives data producers the assurance that their data and associated materials will be stored in a reliable manner and can be reused. It provides funding bodies with the confidence that data will remain available for reuse and their investments will not be lost. It also enables data consumers to assess repositories where data are held and supports data repositories in archiving and distribution data efficiently.

The reason for choosing the Materials Cloud data repository is multifarious: First, the Materials Cloud data base is specially dedicated to **Computational Materials Science**, a subdomain which exactly matches the conducted mathematical modeling performed here. Second, this data base complies fully with the FAIR principles as it offers a FAIR and long-term storage data repository of research data in the areas of computational materials science, engineering, theory and modelling. Herein, the focus is placed primarily on sharing the full provenance of the calculations, while Digital Object Identifiers (DOIs) are being assigned to make the provided data persistent, unique, easily discoverable and citable, thereby adhering fully to the FAIR principles for scientific data management. Third, submission and maintenance of records on this data base is completely free of charge and only subject to some general rules for submission related to overall format and structure of uploaded data. Fourth, the submission process on this data base is straightforward requiring the completion of a form with the research data and metadata. Fifth, Materials Cloud archive uses a DSA indicating a good trustworthiness of the repository. Finally, this data base is Swiss-based, run and maintained by EPFL-associated groups, thereby providing reassurance of a safe storage of data, as well as advertisement and efficient usability of local Swiss facilities and resources.

4. Implementation of FAIR principles

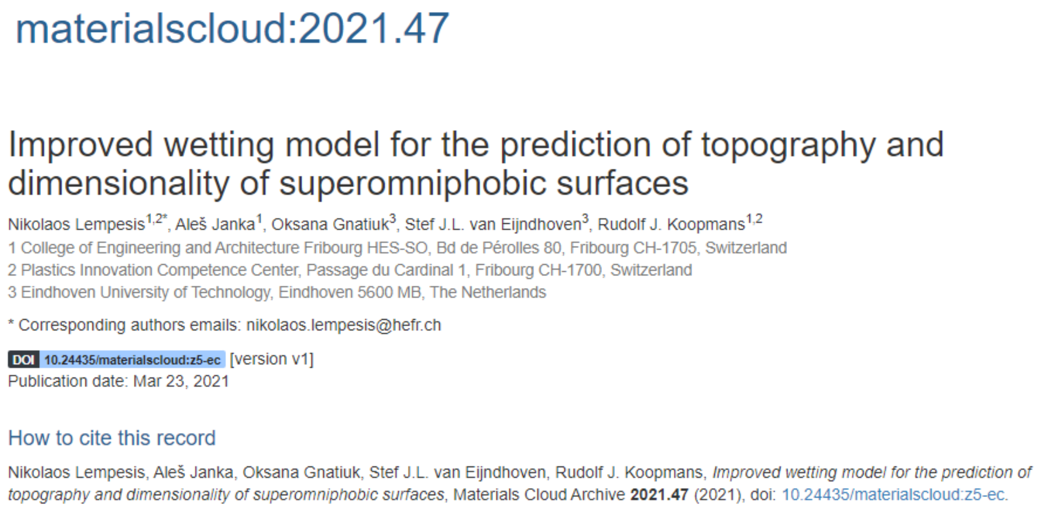
We agree with the general principle that research data originated and/or generated within publicly funded projects should be freely and effortlessly accessible to the general public, as well as to more specialized recipients. The benefits of adopting such a doctrine are multifold. Firstly, by making project data adhering to the FAIR principles, that is findable, accessible, interoperable and reusable, helps in promoting and advancing science in a faster and more efficient way. Scientists from all over the world may access the data and benefit from it both in terms of saving time and in terms of sparing the trouble to solve something already addressed. In addition, FAIR principles ensure a good and efficient knowledge dissemination, promoting thus didactic and educational actions, that otherwise would have been more laborious, if not impossible. In line with that, sharing the results of this project in an Open Data repository fosters scientific and technological advancement very efficiently.

The completion of the goal of this project, which is related to designing superomniphobic surfaces, helps in the development of better packaging materials and storage units for food, water and other edible everyday commodities, thereby offering enormous societal benefits related to proper management and consumption of food and water resources.

Besides the obvious product loss problem, adhesion of food to packaging materials is directly associated with poor product appearance and increased package recycling costs. Moreover, in industrial plants, product adhesion to machinery is responsible for increased surface-cleaning costs. Therein, two significant side effects of microscopic soiling of plant equipment are related to sanitary problems and production deterioration, both in terms of quality and quantity, due to fouling. Hence, proper design of superomniphobic surfaces leads to economizing exorbitant expenses, thereby showing the vast economic impact of this project on reducing recycling costs and machinery maintenance. Applications related to improved flowability of solid bodies within water owed to reduced friction and improved buoyancy showcase vividly the very promising potency of the developed technology for energy saving, thereby highlighting the prominent environmental impact of this work.

The steps followed to adhere to the FAIR principles included the usage of non-commercial and/or open source software tools, such as Notepad++ as text editor for the creation of freely accessible and editable csv text files. Executable files or instructions how to generate them of codes for different types of operating systems (Windows, Linux/Unix, MacOS) were included to accommodate all sorts of working environments. The necessary skills to access, read/edit and run the included files are minimal reducing to the usage of a simple text editor to open/read/write the documentation files and any operating system among Windows/Linux/MacOs. Most importantly, the used data repository (Materials Cloud Archive) is very easily accessible, while it assigns DOIs to the uploaded data set, thereby making it persistent, unique, easily discoverable and citable adhering fully to the FAIR principles for scientific data management. The work time dedicated to the conversion of generated data into a FAIR-compliant format, the uploading process to the data repository, as well as the subsequent processes of reviewing and revisioning until final approval amounted to three weeks. An additional week was dedicated to drafting and finalizing the current report in full compliance to the project call objectives.

In Figure 1, representative snapshots are shown of the created data record on Materials Cloud Archive. The assigned DOI is as follows: 10.24435/materialscloud:z5-ec, while the name of the uploaded file is "Improved wetting model for the prediction of topography and dimensionality of superomniphobic surfaces".



materialscloud:2021.47

Improved wetting model for the prediction of topography and dimensionality of superomniphobic surfaces

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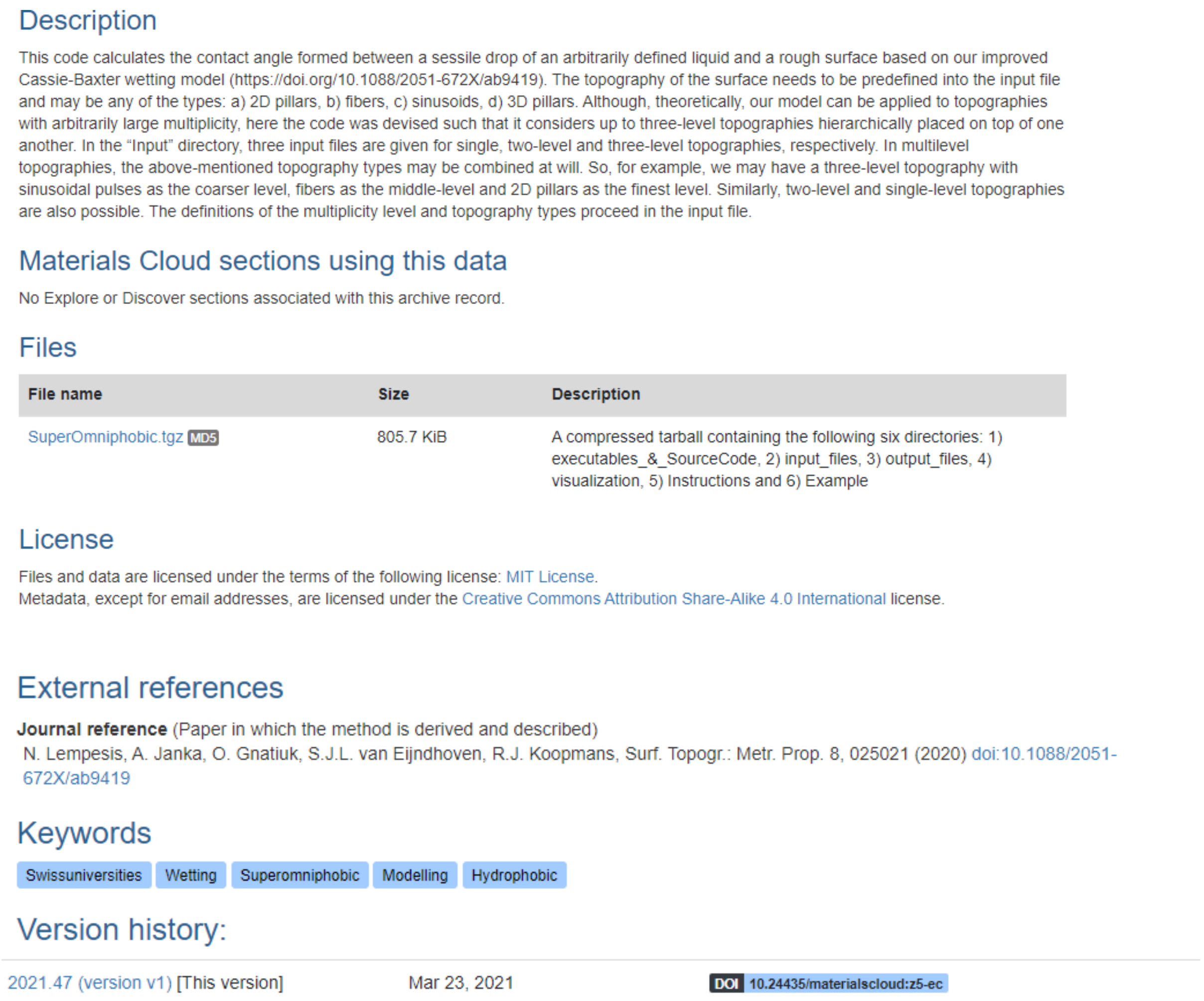
DOI 10.24435/materialscloud:z5-ec [version v1]
Publication date: Mar 23, 2021

How to cite this record

Nikolaos Lempesis, Aleš Janka, Oksana Gnatiuk, Stef J.L. van Eijndhoven, Rudolf J. Koopmans, *Improved wetting model for the prediction of topography and dimensionality of superomniphobic surfaces*, Materials Cloud Archive **2021.47** (2021), doi: 10.24435/materialscloud:z5-ec.



Description

This code calculates the contact angle formed between a sessile drop of an arbitrarily defined liquid and a rough surface based on our improved Cassie-Baxter wetting model (https://doi.org/10.1088/2051-672X/ab9419). The topography of the surface needs to be predefined into the input file and may be any of the types: a) 2D pillars, b) fibers, c) sinusoids, d) 3D pillars. Although, theoretically, our model can be applied to topographies with arbitrarily large multiplicity, here the code was devised such that it considers up to three-level topographies hierarchically placed on top of one another. In the "Input" directory, three input files are given for single, two-level and three-level topographies, respectively. In multilevel topographies, the above-mentioned topography types may be combined at will. So, for example, we may have a three-level topography with sinusoidal pulses as the coarser level, fibers as the middle-level and 2D pillars as the finest level. Similarly, two-level and single-level topographies are also possible. The definitions of the multiplicity level and topography types proceed in the input file.

Materials Cloud sections using this data

No Explore or Discover sections associated with this archive record.

Files

File name	Size	Description
SuperOmniphobic.tgz MD5	805.7 KiB	A compressed tarball containing the following six directories: 1) executables_&_SourceCode, 2) input_files, 3) output_files, 4) visualization, 5) Instructions and 6) Example

License

Files and data are licensed under the terms of the following license: MIT License.
Metadata, except for email addresses, are licensed under the Creative Commons Attribution Share-Alike 4.0 International license.

External references

Journal reference (Paper in which the method is derived and described)
N. Lempesis, A. Janka, O. Gnatiuk, S.J.L. van Eijndhoven, R.J. Koopmans, Surf. Topogr.: Metr. Prop. 8, 025021 (2020) doi:10.1088/2051-672X/ab9419

Keywords

Swissuniversities Wetting Superomniphobic Modelling Hydrophobic

Version history:

2021.47 (version v1) [This version]	Mar 23, 2021	DOI 10.24435/materialscloud:z5-ec

Figure 1: Representative snapshots of the uploaded record on the Materials Cloud Archive data repository (10.24435/materialscloud:z5-ec) adhering to the FAIR principles.

5. Legal and/or ethical issues

We herewith confirm that we are not bound to any partner by a confidentiality clause applicable on any part or the entirety of the data.

We also confirm that the project does not contain any sensitive data, while the right and permission to access the data will be total, i.e., there is no controlled access, nor is there any embargo period.

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