Simulating Nonlinear Nano-to-Micro Scaled Material Properties and Effects at the Architectural Scale

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Abstract

The problem of simulating atypical and nonlinear nano-to-micro scaled material properties at the architectural scale is untenable given the complexity of calculating such data using current rendering and simulation platforms. Though existing rendering engines enable the simulation of material optical properties such as angle dependence, transparency, translucency, and color, the unique behavior and scale of many nonlinear nano materials' angular dependence and wavelength filtering properties requires the development of new tooling methods and workflows. *eSkin*-a project to develop passively responsive building façade systems, frames the larger foundation for this paper, which is narrowly focused upon our catalogue of tools where desired optical properties of nano & micro array structures are first simulated in order to extract angle and wavelength dependent quantitative optical data. Once calculated, these optical properties are then redeployed at the architectural scale utilizing custom written software platforms and algorithms.

1. INTRODUCTION

1.1. Background on eSkin

As part of the *eSkin* project, the work presented in this paper is one subset of ongoing trans-disciplinary research spanning across the fields of cell biology, material science, electrical and systems engineering, and architecture. *eSkin*, the full title of which is, *Energy Minimization via Multi-Scalar Architectures: From Cell Contractility to Sensing Materials to Adaptive Building Skins,* is jointly housed at the University of Pennsylvania and Cornell University. The PIs on the project are: Shu Yang, Jenny E. Sabin, Nader Engheta, Jan Van der Spiegel and Kaori Ihida-Stansbury. Andrew Lucia is Senior Personnel. This project represents a unique avant-garde model for sustainable and ecological design via the fusion of the architectural design studio with laboratory-based scientific research. In turn, this project benefits a diverse range of science and technologies, including the construction of energy efficient and aesthetic building skins and materials. Given the groundbreaking nature of this work, many of the tools we use to simulate, visualize and model nonlinear nano-to-micro scaled material properties and effects at the architectural scale must be custom written and designed. While there are commercially available software packages for optical engineering and design such as TracePro that can handle some, but not all of our needs in terms of angular and spectral dependent properties, our interest resides in developing a design process to work with these nano to microscaled material features through the development of custom-written tools. Through the development of our own simulation tools that work directly with these optical data while also understanding the state of the art in optical engineering and design simulation, it is possible to generate a thinking space and design intuition for materiality not yet realized at the architectural scale. To this end, this paper focuses on our latest set of visualization and design tools.

Comprised of a field of low cost sensors and passively responsive materials, eSkin is conceived to be generic and homogenously structured upon installation (i.e. laden with the full potential) but readily adaptable to local heterogeneous spatiotemporal conditions, thereby reducing the overall functioning demands upon it and ultimately lowering overall energy consumption. In this regard a "learning" and adaptive second skin would forgo the need for lengthy, costly, and one-time site analysis relegating ever changing environmental analysis and response of the local and global spatiotemporal environments to its own internal/local functionality. This manner of operation not only maximizes immediate performative efficiency, but also allows for ongoing contextual adaptation.

Ultimately the goal of the eSkin project is to explore materiality from nano to macroscales based upon understanding of nonlinear, dynamic human cell behaviors on geometrically-defined substrates. Through the eSkin project, insights as to how cells can modify their immediate extracellular matrix (ECM) microenvironment with minimal energy and maximal effect are being investigated and applied to the biomimetic design and engineering of highly aesthetic, passive materials, and sensors and imagers that will be integrated into responsive building skins at the architectural scale.

1.2. Background on materials research & challenge

The particular research presented in this paper focuses on one subset of study within the eSkin project, the optical simulation and application of nano-to-micro scale PDMS pillar array substrates (Figure 1) deployed at the building scale. Specifically, these nano/micro scale pillar substrates, designed in the Yang lab, form the basis of this investigation. These substrates are fabricated via microlithography and softlithogragy, first requiring a negative nano/micro pattern to be etched into a substrate in which PDMS is subsequently cast, cured, and removed, thus producing a positive relief of nano/mico pillars (see for example Thompson et al. 1994, Xia et al 1998, & Zhang et al. 2006). Though these positive substrates may be cast using an array of polymers, compounds and mixtures, for the purpose of this study we are exclusively interrogating the properties of PDMS as a proof of principle.

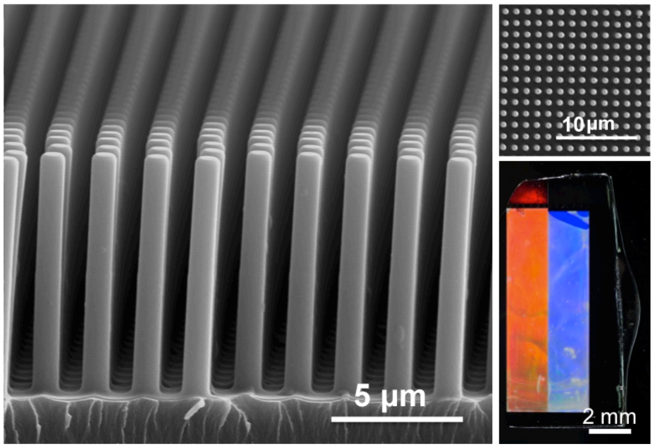


Figure 1. SEM image of square micropillar array (left). Photo Credit: Lo, C.W., Zhang, Y., and Yang, S., Univ. of Pennsylvania. SEM (upper right) and optical (lower right) images of micropillar arrays. Two different colors (lower right) result from Bragg diffraction of micropillar arrays with different periodicities (image adapted with permission from from CHANDRA, D., et al. 2009. Biomimetic ultrathin whitening by capillary force induced random clustering of hydrogel micropillar arrays. ACS Appl. Mater. Interfaces. Vol. 1. No 8. 1698–1704. Copyright 2009 American Chemical Society).

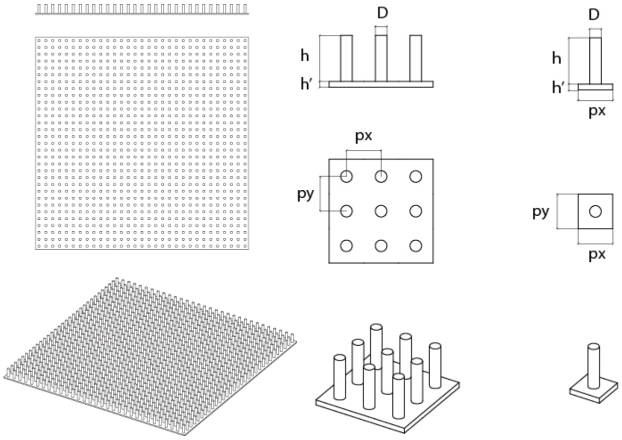


Figure 2. Left, schematic geometry of nano/mictopillar arrays. Right, schematics of nano/micropillar units.

Demonstrating unique angle dependent and wavelength filtering optical properties of interest, these periodic pillar arrays act as passive filters of light given the specific nano or micro scale periodicity of their structures and the angle at which they are viewed. Because of the particular periodic spacing and geometry of these arrays existing at the nano-to-micro scale, light is absorbed via the PDMS material, but also filtered as a property of the particular wavelength of light that is allowed to pass through a particular pillar array. Depending on factors such as the diameter and the periodic distance between each pillar in an array, the visible spectrum of light, which exists between 390nm to 750nm, will be filtered out, absorbed/scattered, or reflected/refracted from the material (Figure 3).

Though these qualities can be seen by the naked eye (Figure 1), extracting their optical performance quantitatively for speculation at larger architectural scale applications is necessary given a.) the current limitations in which these substrates can be fabricated (currently 4 inches maximum), and b). the necessity to speculate on large scale deployments of potential materials without the need to actually fabricate. Thus, simulating the effects of larger swathes of these materials has been a goal and focus of this research; to speculate as to the larger scale application and effect of these substrates in an architectural context.

Aside from the unique angle dependent and wavelength filtering properties foreign to many existing architectural simulation and rendering software (exceptions discussed below), there exist more fundamental modeling and memory issues that do not allow for the explicit modeling and simulation of nano/micro scale materials at the architectural scale. Though it would be conceivable to geometrically model large swathes of these structures using existing software, overcoming limitations of computational memory is a major obstacle. The amount of memory necessary to deploy vast arrays of nano scaled features in an architectural context is inconceivable and several orders of magnitude beyond current standard capabilities. For example, the memory requirement to model and distribute a cylindrical nanopillar (D = 200nm & h = 800nm) with 400nm periodic spacing of 100 x 100 units (40um x 40um total sample size) approaches 290mb in NURBs, 750mb in refined mesh, and 96mb in low-quality mesh. Extrapolating further, a 10m x 3m swath of this same modeled material would be 1.76*10^9 gigabites in even low-quality mesh. Thus, modeling large swathes of these nano materials at an architectural scale is highly impractical.

Even if this were overcome, a second limitation exists given the current state of simulation and rendering software, namely that most platforms do not take into consideration the filtering of angle dependent wavelength data through material at the nano/micro scales. A few exceptions do exist, however, but are limited for our purposes. One robust exception to this limitation is the software TracePro by Lambda Research, which uses geometric optics as a basis for its simulations. While TracePro does take into consideration angle dependent geometric optics for specular material, BSDF (bidirectional scattering distribution function), or a combination of both, its current capabilities do not account for sub-10 micron feature sizes or wavelength filtering at this scale, which are specific material properties of interest to our research. Maxwell, another popular and highly accurate software for design rendering, is limited for our purposes in that only color with incident angles of 0 degrees and 90 degrees are taken into consideration. Here again, our research demands the full range of angle dependent behavior between these poles. Another option, Radiance, can simulate angle dependent properties but is not specialized or suited for rendering complicated geometric surfaces, and only capable for rendering pure BSDF or specular material.

The unique properties generated by certain nanoscale materials, such as those we are probing, require new approaches to workflow in our tooling environments as we venture into a new era in which we are capable of actively influencing material properties at the nano scale. Architects have always engaged materiality in the design process. Our challenge is to develop a design process and material inuition through the crafting of digital tools that simulate material properties that cannot be engaged directly with the hand or in some cases, the naked eye. In order to overcome this design and visualization challenge, we have developed a methodology and workflow by which the nonlinear optical properties of these nano materials are simulated for a small portion of an actual sample, and then distributed across vast macro areas through the use of custom written algorithms in conjunction with robust rendering engines.

2. METHODS

First, the unique physical and angle dependent optical properties of a small portion of these periodic geometric substrates are simulated in the labs of Van der Spiegel and Engheta through the use of Lumerical FDTD Solution, a material simulation software. Due to the periodic nature of the substrates in question, only a portion of these substrates need be simulated, after which the characteristics of the material would "repeat" itself. These simulations, which derive the angle dependent optical properties of the material substrates, ultimately form the basis for larger scale simulations of potential material applications within the eSkin system. At the architectural scale, speculations as to the extracted performative and aesthetic qualities of these nano/micro materials are then deployed using custom written algorithms in conjunction with the Rhinocerous (NURBS modeling) software environment.

2.1. Simulating Optical properties at the Nano-Micro Scale

As stated prior, the nano/micro structure tested in simulation is a periodic high-aspect-ratio (HAR) pillar array. To simulate these pillar arrays with high efficiency, a simplified geometry is necessary to begin with. First, a matrix of pillars and a continuous sheet of substrate are modeled as a NURB surface and mesh.

As illustrated in Figures 1 & 2, the structure of the untreated pillar substrate is 2D periodic. Therefore, the optical properties of the pillar array may be obtained by simulation of a single unit in a matrix. While neighboring units must be considered, immediate neighbors in the simulation are taken to be the same geometry in order to increase efficiency. The parameters that describe the geometry of such units are shown in Figure 2, where the aspect ratio of the micropillar is AR: AR = h/d. This periodic structure is the simplest condition of the substrate, excluding any variation or gradient across the field of pillars. Any reshaping or treatment method that destroys the periodic property of the epoxy micropillar arrays cannot be analyzed by this method, but is being considered for future investigations.

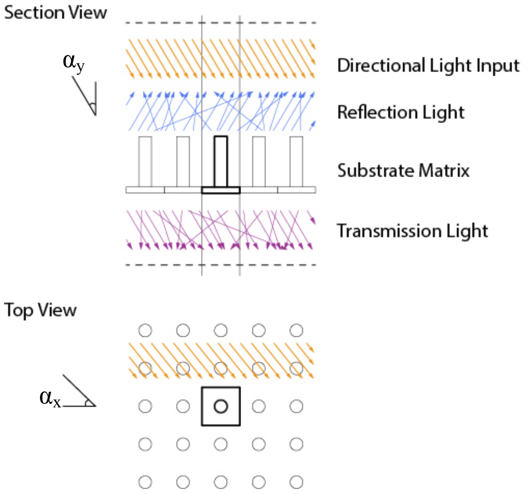


Figure 3. Two sub directions of incident light and reflection and transmission light.

To develop a digital material that reproduces the optical properties of the selected sample faithfully, its bidirectional light distribution function must first be determined in transmission (BTDF) and reflection (BRDF), so that the spatial distribution of emerging light can be identified for varying incident directions. For this simulation we use Lumerical FDTD Solution, specifically designed for determining nano-scale optical effects. The process of simulation can be described as follows: a light source with intensity, I, at given incident angle, α, is evenly distributed. Total light intensity coming from reflection by the substrate will be recorded as I_r, that from transmission is I_t. The reflection coefficient, C_r, and transmission coefficient, C_t, are:

$$c_r = I_r/I$$

$$c_t = I_t/I$$

Since the only power source is the incident light, the summation of C_r and C_t should be equal or less than 1.

Because the scale of the pillar array nanostructure is very close to visible light wavelength, the material is highly sensitive to different light wavelengths, λ, at different incident angles, α. The variable α in this case can be interpreted as the angle between the light direction and substrate surface normal, α_y, and the angle between the light direction in the substrate surface and matrices direction, α_x. To fully understand the optical properties of the material, the incident light must be considered in different directions with different α_y, and α_x. Given the symmetrical and periodic property of the matrices, only ½ α_y and 1/8 α_x are necessary for simulation (Figure 5, a & b). Taking into consideration these varied directions with respect to a sphere, it is only necessary to calculate 1/16 of the sphere as shown in Figure 5c. Simplifying the simulation process, α_y' can be defined as the angle between the surface normal facing the light source. α_x' is the smallest angle between 2 major matrix direction lines as illustrated in the following diagram (Figure 4). The domain of α_y' is [-90°, 90°]. That of α_x' is [0°, 45°].

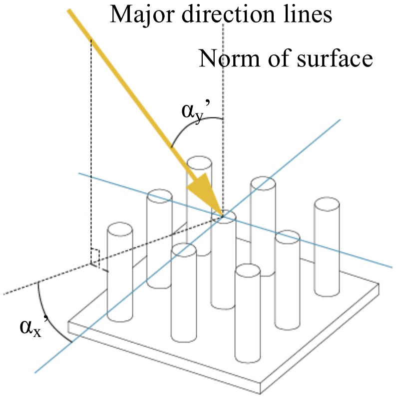


Figure 4. α_x' and α_y' incidental angles

Since the material is wavelength sensitive, it is necessary to obtain a spectral power distribution for both reflection,

$I_r(\lambda)$, and transmission light, $I_t(\lambda)$, at each light angle. Given the spectral power distribution of input light, $I_i(\lambda)$ where $C_r(\lambda)$ and $C_t(\lambda)$ are reflection and transmission coefficients at a specific wavelength λ (Fairchild, 2005):

$$I_r(\lambda) = c_r(\lambda)\ I_i(\lambda)$$

$$I_t(\lambda) = c_t(\lambda)\ I_i(\lambda)$$

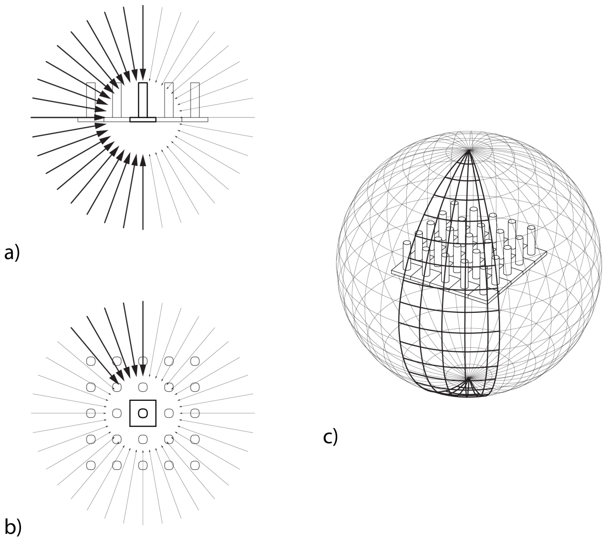


Figure 5. Simulation of the incident angle about a sphere

As opposed to conventional architectural material simulation and rendering software, the direction of reflected and transmitted light of these unique nonlinear nano/micro pillar surfaces and substrates perform neither like a conventional specular surface, nor a diffuse material. To this end, our method requires integrated spherical measurements rather than a total summation of reflection light and transmission light intensity in all directions.

From this nano/micro material simulation, we are able to obtain the reflection and transmission coefficient of the material under specific light incident angles (including α_x and α_y) given unique light wavelengths.

2.2. Interpreting the Simulation Data

Methods for interpreting large amounts of simulation data are key for simulations operating at the building scale and in understanding the optical properties of the nano/micro material in architectural contexts. Light in the natural world is almost never purely monochromatic. To analyze or simulate our virtual material substrates under polychromatic light mixtures, the following process has been developed.

2.2.1. Obtain XYZ value via color matching function

$I_r(\lambda)$ is the reflected spectral power distribution. For a single light source:

$$I_r(\lambda) = C_r(\lambda) I(\lambda)$$

Similarly,

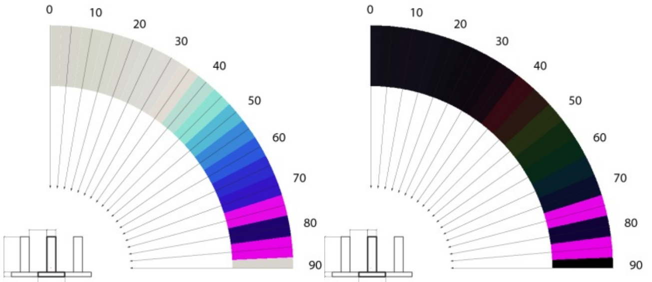
$$I_t(\lambda) = C_t(\lambda) I(\lambda)$$

For multiple light sources (n), at a certain wavelength (λ), the overall reflected/transmitted spectral power distributions are:

$$I_r(\lambda) = \sum_{i=1}^{n} C_{ri}(\lambda) I_i(\lambda)$$

$$I_t(\lambda) = \sum_{i=1}^{n} C_{ti}(\lambda) I_i(\lambda)$$

Thus, through the color matching function, the reflection color, and transmission color of the substrate can be calculated (Vos, 1978 & Wyszecki, 1982). An example of the unit simulation was conducted to show the method. The unit for this test has the following parameters: D = 200nm, AR = 4, h = 800nm, Px = 400nm, & Py = 400nm. Given this, the simulation was processed from 0 to 90 degrees by 5 degree increments with a “middle resolution” mesh generated from NURBs surface and implemented using a custom written algorithm written in Grasshopper. Figure 6 shows the reflection color and transmission color calculated by the algorithm based on the method described in 2.1 versus incident light angle.



(a) (b)

Figure 6. Reflection (a) and transmission (b) color versus incident angle (α_x) of the sample test.

As illustrated in Figure 8, visible color change for this sample happened after the 35 degree incident angle. After 75 degrees, the color of both reflection and transmission become very unstable. This issue will be addressed in future iterations. Ideally, data shown in Figure 6 should be tested for each α_y. For this paper, the discussion was limited to α_x from 0^o to 90^o. For the particular material tested in this proof of principle, given an increasing incident angle, the material tends to be more transparent /translucent.

Having interpreted the nano/micro scale simulation data, we may now deploy these optical and material properties at the architectural scale.

2.3. Simulation and Rendering at the Architectural Scale

Given that there is no software available to render faithfully the types of materials under consideration in this study, the large-scale deployment and simulation of these material effects must also be a part of our custom digital tool kit. In order to overcome this, the quantitative values of simulated material properties from the above method are considered across large-scale surfaces via custom written digital tooling methods and algorithms. For the purposes of this study, these tooling methods have been carried out in Rhinocerous, utilizing the Grasshopper Plug-in. Due to shortcomings of these architectural rendering and modeling environments, however, Rhino/Grasshopper will not directly render the material. The level of scripting freedom embedded within tooling components in these software, however, does enable one to write custom algorithms that are close and efficient approximations of the nonlinear material properties inherent to the tested nano/micro substrates. This allows a seamless connection with modeling software, making it possible to produce real-time visualizations and ultimately prepare material for robust rendering using software such as Maxwell.

3. RESULTS

As mentioned before, a vast amount of data is obtained by simulation. Measured data is organized in the following format to be analyzed:

Λ	$C_r(\lambda)$	$C_t(\lambda)$
780	0.882837	0.11386
767.005	0.880057	0.116441
764.0299	0.87806	0.118748
761.0744	0.876797	0.120779
758.1384	0.876158	0.122527
…	…	…
380	0.712232	0.282342

Table 1: Reflection/transmission coefficient at different wavelength, $C(\lambda)$, and spectral power distribution function of input color, $I(\lambda)$.

For a single surface with a single light source of uniform distribution, each point on the surface has the same optical properties. Therefore, evaluation of the center point represents properties of the whole surface. With one single light, the two sides of the surface can be named as the reflection side and transmission side. After calculating the redefined incident angle (α_x'), and angle between the light source and pillar matrix direction (α_y'), a matrix of C_r and C_t at different wavelength (λ) can be obtained by interpreting the measured data. For a given light source with a specific spectral power distribution ($I(\lambda)$), reflected/transmitted spectral power distribution can be obtained by $C_r(\lambda)\ I(\lambda)$, and $C_t(\lambda)\ I(\lambda)$, so that the previously discussed method can be used to generate a XYZ color for the surface. With multiple light sources, a total reflection/transmission spectrum has to be calculated by the previous equation. Finally a color in XYZ space can be generated based on the color matching function. To represent the different behavior of both sides of surfaces, the surface was offset minimally in both directions with a small distance (Figure 7).

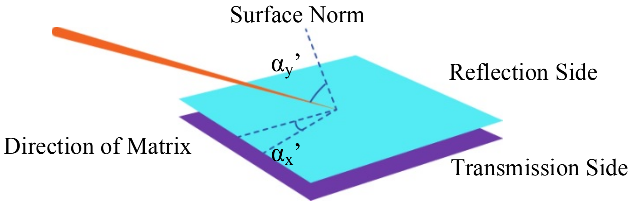
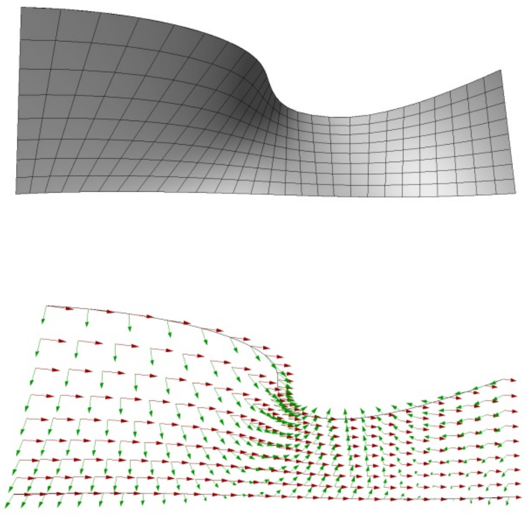


Figure 7. Incident light angle on two sides of a surface

For a curved surface and/or uneven distribution of light, the analysis of a sub-divisional surface is necessary. Having sub-divided the larger surface into a number of small discrete flat mesh sub-surfaces, we are then able to run the simulation for the vertex of each sub-divided face and linear interpolation colors are assigned by mesh color properties to approach the overall property of the surface. As before with the use of a flat surface, the basic logic is to turn a NURBs surface into two meshes with a small distance between each. This replicates a double-side property of the material, one for reflection and one for transmission. Furthermore, since the mesh is uniquely colored at each vertex, the process of simulation for single curved surface with uniform light has to be conducted for each sub-divided vertex comprising the whole. The following drawings show the process under a uniform directional lighting condition (Figure 8).



a.

b.

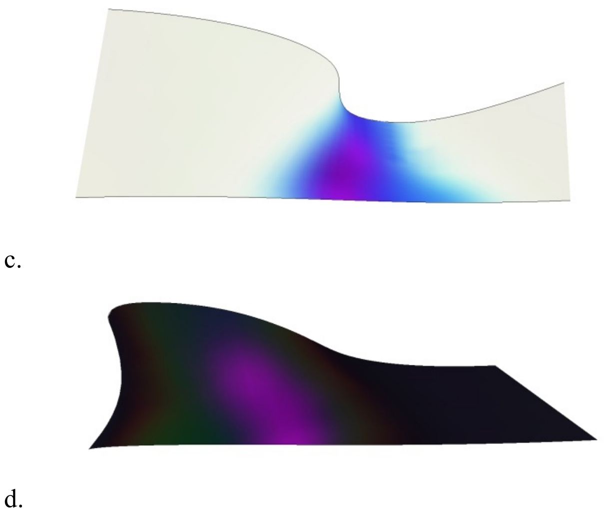


Figure 8. a) Mesh from NURB surface; b) Direction of matrix and surface normal of each vertex; c) Colored mesh (reflection side) based on described method; d) Colored mesh (transmission side) based on described method.

Having assigned a unique material property to each mesh face across the surface, the final output of this method enables a colored mesh that can be directly rendered by standard architectural/computer graphics rendering software.

For software, such as Maxwell, that does not support colored meshes; a script generates a bitmap, demonstrated in Figure 9, for rendering a diffuse map of a material and a mesh with modified texture mapping coordinates that match the bitmap (How to Render Mesh colors?, 2012).

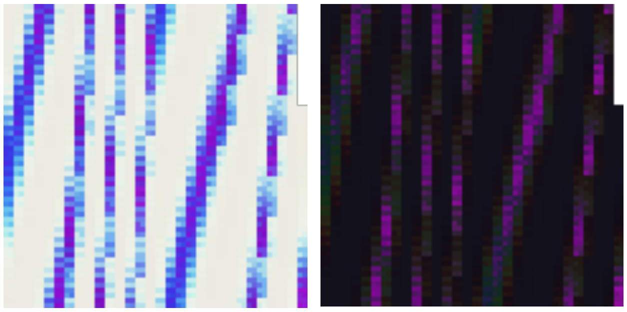


Figure 9. Bitmap for rendering material mapping to both sides of a surface, reflection side (left) & transmission side (right).

The following example (Figure 10) shows a rendered image of a test façade, whereby the color of each panel varies passively, according to the methods described in this paper.

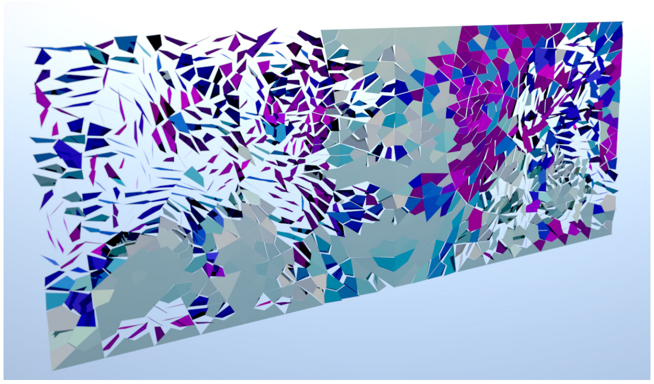


Figure 10. ColorMapping of the test facade by using the method described, and rendered in Maxwell.

4. DISCUSSION

The representation of material and material properties has long been a critical portion of the architectural design process. To illustrate or render is to convey intention behind a particular set of spatio-material ideas. From the pen to the computer, architects and designers have sought and implemented tools to aid in this visually communicative endeavor. Though advances in computer graphics have afforded the ability to speculate and render complex material environments with extremely accurate and realistic models of light based on reflection, refraction, scattering, and diffusion, these environments are, by and large, comprised of stable "architectural materials," which have until now comprised a pallet of materials whose properties one might consider consistently deployable over large swathes of surface without a deviation in their phenomenal behavior.

Through the collaborative efforts embarked on within the *eSkin* project, an identified point of impasse arose when the issue of propagating/rendering a simulation of unique observational and wavelength dependent nano/micro scaled material was to be emulated and speculated upon at the architectural scale. More specifically, the materials of interest exhibit nuanced nonlinear behavior as a product of their nano and micro scale geometric structures, such as angle and wavelength dependent properties. This, in turn, led to an investigation that extracted the quality of these properties, while at the same time eliminating the need to geometrically model *ad infinitum* these nano/micro materials across an architectural scaled application. Even if the latter were computationally possible, the current state of rendering technologies is not sufficient for simulating optical and light based properties at the fine-grained scale required of the materials in question. Save uniform material attributes of refraction, reflection and transmission, current rendering technologies do not take into consideration many of the combined unique nanoscaled material properties queried in this paper, including surface curvature, points of observation, discrete wavelength filtering, and the effect of multiple points of incident light.

Though several issues persist as unresolved future areas of exploration within this study, the methods presented here demonstrate a working methodology for dealing with the effects of nonlinear nano/micro differentiated materials; materials whose properties are dependent on several parameters not typically associated with common macro materials. Whereas common linear materials that are mapped or "applied to surfaces" in a rendering environment devoid of a particular scale (i.e. the object is red, has x refraction, and x transmission), these nonlinear nano/micro scaled materials explored in this study must not only be attributed in a scale specific manner, but also with a sensitivity to the direction in which an observer may "see" the material. This also implies a unique qualitative signature that is intrinsically aligned with the morphology of a surface.

5. CONCLUSION

Advances in materials science are rapidly advancing the ways in which architects may "see" and design their material environments. Once, limited to a material pallet comprised of matter that was largely conceived of and affected by consistent notions of light intensity, direction, shadow, macro applied color, and the like, we are now forced to deal with an artificial world that no longer behaves according to well established norms of "common" material phenomenal properties. While the interplay of light on a steadfast architectural material such as steel, brick, wood, stone, and glass, has produced incredible phenomenal results throughout history, we are now forced to deal with a new reality of a customizable and tunable material world, one in which we are capable of actively defining as architects.

The implications of current material technology advances and the speculative approach outlined in this paper not only implies, but deploys a notion that affect is generated through the articulation of form, rather than merely being applied to a shape or morphology after a "design" has been executed. The latter is the common practice of workflow given current rendering technologies and modes of design thinking. In our case, geometry, matter and associated optical effects are embedded and contribute to the design and simulation process across multiple length scales. This is not just about overcoming technical gaps that exist in robust commercially available optical engineering and design softwares, but most importantly is about contributing to and fostering a design space saturated in materiality. By designing custom-written tools to simulate nano to microscaled material properties and interfacing these related data directly, it is possible to develop design intuition for materiality not yet realized at the architectural scale. The approach outlined in this paper underscores the importance underlying the generation of affect being intrinsically linked to observation and material organization, rather than through the *ex-post facto* application of materiality and effect to predefined shapes.

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