TUNABLE DIGITAL MATERIAL PROPERTIES FOR 3D VOXEL PRINTERS

Jonathan Hiller, Hod Lipson
Mechanical and Aerospace Engineering
Cornell University
Ithaca NY, USA

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Abstract

Digital materials are composed of many discrete voxels placed in a massively parallel layer deposition process, as opposed to continuous (analog) deposition techniques. We explore the material properties attainable using a voxel-based freeform fabrication process and simulate how the properties can be tuned for a wide range of applications. By varying the precision, geometry, and material of the individual voxels, we obtain continuous control over the density, elastic modulus, CTE, ductility, and failure mode of the material. Also, we demonstrate the effects of several hierarchical voxel "microstructures", resulting in interesting properties such as negative poisson's ratio. This implies that digital materials can exhibit widely varying properties in a single desktop fabrication process.

Introduction

Digital, (discrete) materials are fundamentally different from analog (continuous) materials. Digital materials break up 3D space into a series of 3D pixels, which are either occupied by a voxel (instantiated piece of material) or left vacant. This paradigm (Gershenfeld, 2005) allows all the advantages of the digital realm such as perfect repeatability and error correction to be realized in a physical 3D object. This approach fundamentally works for any number of materials, enabling multi-material composite objects, as opposed to many other SFF processes limited to a single material per build (Kadekar *et al*, 2004). Although voxels are routinely used as a data structure in computer graphics, (Chandru *et al*,1995) and even to prepare models for conventional freeform fabrication (Lin *et al*, 2007), here we refer to them as physical bits in digital matter.

Digital materials may be broken into two classes: The first involves accurate placement of drops of material which harden in place. These droplets, often jetted from an inkjet system (Calvert, 2001) may be of multiple materials, but are limited in their rheological properties and must be placed very precisely to maintain a true digital solid. Machines using this technique are commercially available (Objet, 2008) and produce excellent parts with regions of varying materials properties. Other multi-material freeform fabrication systems exist capable of printing many different materials (Malone *et al*, 2004), but are not well suited for creating composite materials, and are also limited in the rheological properties of material which can be processed.

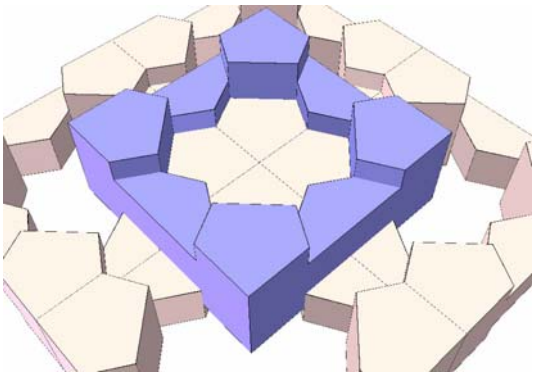
The second class of digital materials, which will be address in the work presented here, involves assembling pre-fabricated voxels. (Popescu *et al*, 2006a, 2006b) These voxels

may be of any geometry, but they ideally self align upon assembly. In this case, the overall accuracy of the digital solid is determined by the individual voxels. (Hiller and Lipson, 2008) Because the fabricator need only place the voxels within their region of self alignment, it can produce objects more accurate than its own positioning system. Additionally, any material that can be formed into the desired voxel geometry and is solid at the processing temperature is compatible. Voxels may take the form of spheres, which are easy to manufacture and have a large region of self alignment, or more complex interlocking shapes which do not require post-processing to bind together.

Background

In order to better understand the properties of voxel-based materials, we developed a comprehensive simulation framework to simulate the physical properties of structures composed of thousands of voxels of multiple materials. This framework incorporates non-linear interaction between interlocking voxels including surface contact and plastic material yielding. Also, it supports first order modeling of random variation in tile geometry resulting from non-ideal manufacturing processes and thermal effects. In addition, random half toning between two materials is possible, and user-definable voxel sub-structures (microstructure) that can be tiled throughout a region.

As a case study, we consider interlocking square voxels as presented in Hiller and Lipson, 2008. (Figure 1) These were selected as representative for interlocking voxels and their suitability for mass fabrication at a microscale. Due to the simple 2.5D geometry, this geometry is suitable for fabrication using molding, lithographic, hot embossing, and many other techniques. This enables a wide variety of materials to be used, such as metals, polymers, ceramics, and many others at a wide variety of scales. For instance, metal tiles could be stamped out of a sheet, polymer tiles could be hot embossed, ceramic tiles could be injection molded, and silicon tiles could be etched out of a wafer. Rotation and flip invariance of the design makes them also suitable for a massively parallel digital fabrication process. Although all following results are based on this geometry, the principles demonstrated apply to all voxel geometries that physically interlock.



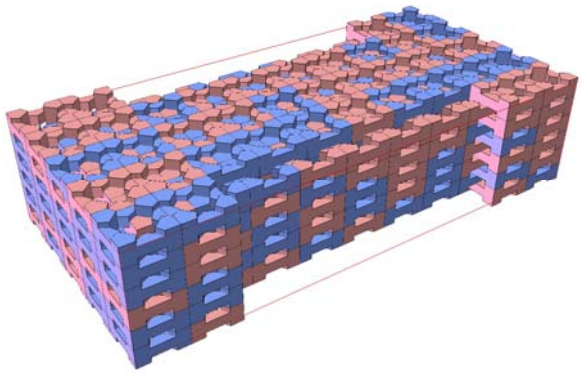


Figure 1: 2.5D interlocking square voxels (left) are considered for this analysis due to their ease of fabrication at many scales/materials. Virtual tensile tests were carried out on large blocks of voxels of multiple materials (right)

A relaxation algorithm (Lipson, 2006) was implemented in order to calculate the rest position of each voxel under random dimensional variation and/or prescribed force or displacement to the structure. The entire simulation was written in C++ for superior speed, flexibility, and the ability to use real-time OpenGL 3D visualization of the structure. Dynamic time stepping was implemented to ensure quick convergence while maintaining computational stability. Running on a single core of a desktop computer, a relaxation cycle of 1000 tiles (10x10x10 block) composed of 4500 individual interactions takes approximately 3ms per time step and scales as O(n) (roughly linearly with number of voxels). Convergence is arbitrarily defined to be when average tile movement is less than 10 picometers for a given timestep. The aforementioned example takes about 1100 time steps to converge, or 4 seconds on a single CPU. This allows us to feasibly compute a statistically significant number of trials for the work presented here.

In order to accurately model the force between each voxel and its neighbors, a finite element model was developed in COMSOL Multiphysics for each type of tile interaction. (Figure 2) In the case of square tiles, this included an in-layer edge-to-edge interaction and an inter-layer corner-to-corner interaction. The materials model was elasto-plastic, and the interaction between the tiles was modeled as a non-linear contact force. Several assumptions were made: First, individual tile interactions were considered independently within a given tile. This does not pose a problem as long as the material has not yielded, but past that point it provides only an approximation of the tile failure. Failure was take to occur as soon as the maximum stress in the tile reached the ultimate tensile stress of the material. This corresponds to the worst case condition, and in reality higher deformations are likely attainable. Also, displacements and rotations out of plane were disregarded, since tile displacements of the tiles were kept small.

With both tiles of a contact pair modeled in COMSOL, one tile was grounded (about its symmetry plane(s) and a prescribed displacement was applied to the other. The model was run using a non-linear solver and the resulting reaction forces and maximum stress was recorded. This was repeated for varying X, Y, and θ_z displacements to fill out a parameter-space. This data was recorded in a lookup table for importing into the main simulation program. Because the time to retrieve a value in an indexed lookup table does not change with the size of the table, the parameter-space can be filled out to arbitrary accuracy without affecting the actual simulation time.

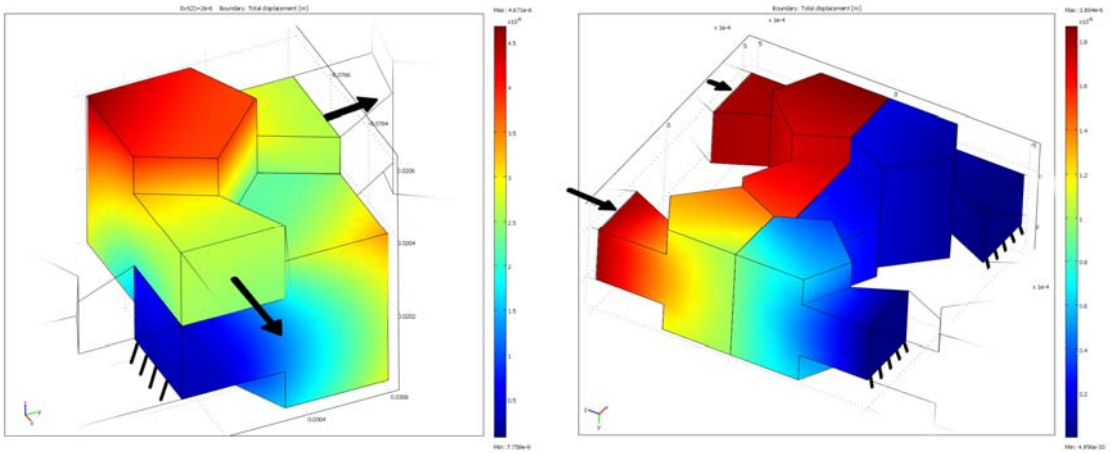
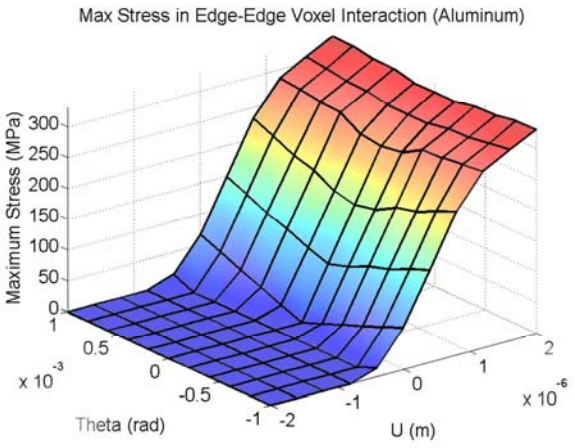


Figure 2: Output of COMSOL finite element simulations for the two types of interactions between tiles. (corners and edges) Interactions were characterized for a range of displacements and imported into a large-scale simulation with 1000's of tiles.

Because of the design of the tiles, there is inherent anisotropy in the Z direction compared to the X and Y. In this direction there is no physical interlocking, just friction that binds the tiles together. Thus, the physical behavior in the Z direction is less interesting, and not addressed in the following results.

Results and Discussion

The results of single tile-to-tile interactions from the finite element modeling are shown in Figure 3 for edge-to-edge and Figure 4 for corner-to-corner interactions of aluminum tiles. The maximum stress plots clearly show the non-linear material model yielding at 276MPa as the tiles are forced into greater interference. The limits of the parameter-space were determined by the displacement necessary to cause the material to reach its ultimate stress.



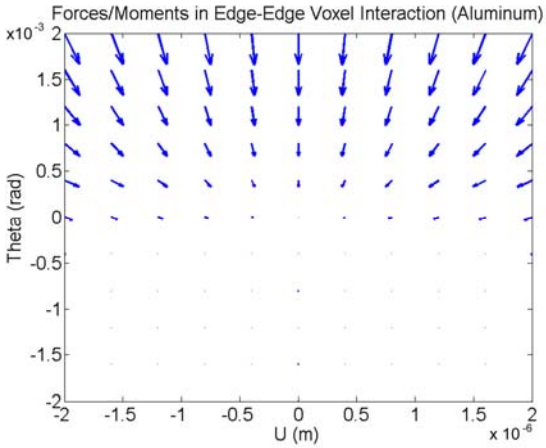


Figure 3: Results of finite element simulations. The stress (left) and resultant forces (right) in edge-to edge tile interactions for a range of tile positions and rotations is shown for aluminum tiles. This info is stored in a lookup table for quick access.

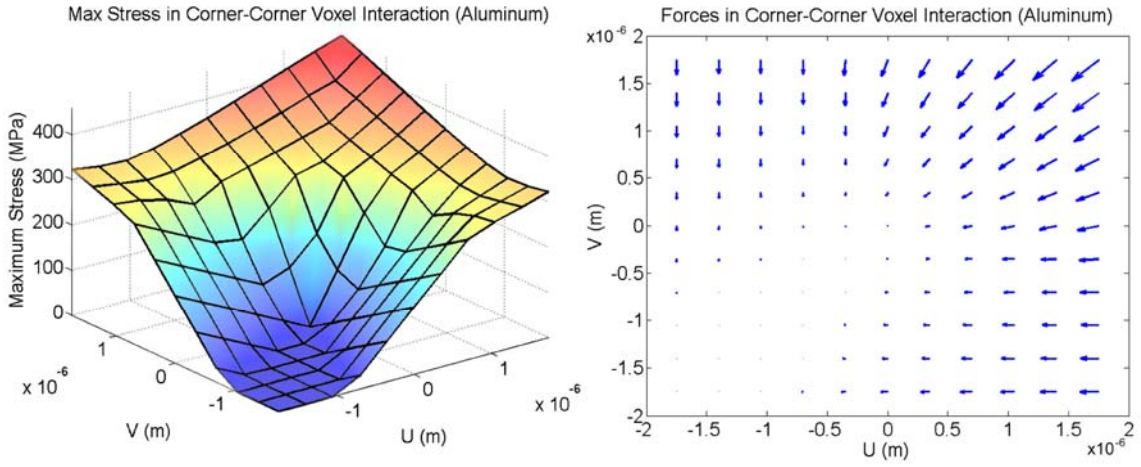


Figure 4: Stress (left) and resultant force (right) for corner-to-corner tile interactions. Each data point represents a separate finite element model solution.

Virtual Tensile Tests

Virtual tensile tests were conducted on structures of approximately 500 tiles, in the configuration shown in Figure 1. As is normal practice in physical tensile tests, the specimen included a slight reduction in area in the center to avoid breakage from boundary conditions at the gripper. The tiles at the extreme ends of the structure were fixed via stiff springs to ground. Multiple relaxation iterations were then carried out, incrementing the elongation slightly each time. The structure was fully relaxed between each iteration, corresponding to a "slow" tensile test, in which dynamic effects are minimal. In the case of one or more joints failing, the relaxation was repeated with the broken joint(s) rendered useless until no more joints broke, in order to allow failure to propagate realistically in brittle samples.

Single Material

As designed, the tiles presented here are space-filling. It is therefore reasonable to compare the material properties of a digital material specimen of a single material to an equivalent sample of bulk (analog) material, which would have equivalent net densities. In the case of aluminum 6061, a bulk elastic modulus of 70GPa was used. In the virtual tensile test, a structure of solid aluminum tiles had an aggregate elastic modulus of 4.75GPa. This corresponds to about a 15x reduction in stiffness. Other materials, such as acrylic, showed similar reductions (10-15x) in overall stiffness.

Even using a single material, the bulk material properties and failure mode of a digital structure can be tuned over a wide range by simply varying the precision of the manufacturing process used to manufacture the tiles. In simulation, this was modeled as a uniformly random variation in the dimension of the tiles over a given range. As the errors

of the tile geometry increased, the elastic modulus continuously decreased and the brittle failure mode became more ductile. (Figure 5) Also, strain to failure increased dramatically, although maximum stress decreased. Additionally, as the voxel error increased, an "uptake" region was introduced in the tensile test, where the slack was being taken out of the structure. This feature can be controlled by the offsets of the tile dimension from nominal, for instance by making all the outside dimensions of the tiles slightly larger.

This brittle-to-ductile behavior is explained by observing the number of failed joints in the structure. When there is greater variation in the voxel dimensions, joints begin to fail before the structure has reached a critical stress. The rest of the structure can absorb the additional force released by the broken voxel, and the number of failing voxels (and thus the failure point of the material) can be predicted. The initial broken joints in the ductile (10μm) case were due to high errors that caused failure upon the original assembly of the structure

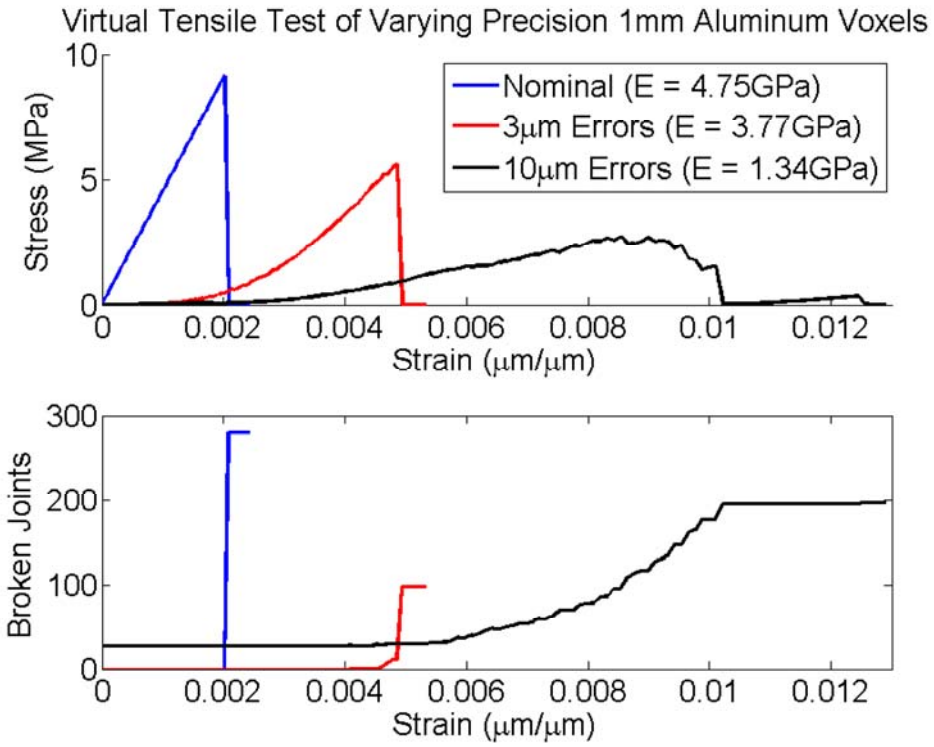


Figure 5: Tensile tests (top) on single material voxel structures with varying precision of the voxel geometries demonstrates a wide range of elastic moduli (E) and failure modes. The number of broken connections (bottom) shows the difference between a brittle and ductile fracture.

Material Half-toning

The properties of digital materials may be tuned even more extensively by introducing hybrid systems of two or more materials. Because a digital fabrication process is inherently compatible with any number of materials in a single build process,

these materials may be easily combined to create hybrid composite materials. The simplest way to do this is to randomly halftone a percentage of two materials to obtain the desired proportions. Much research has gone into half-toning for creating black and white images from grayscale, but for a pseudo-homogenous material, the problem becomes easier. For these simulations, a desired percentage of material was selected. Given the number of voxel in the region to be half-toned, the total number of voxels of each material was calculated and voxels were randomly selected for each material such that the totals added up.

By using this process, bulk material properties of a digital structure may be continuously varied between the properties of each single material. Some properties, such as density, can be calculated analytically based on the percentage and density of the two component materials. For materials of density ρ_A and ρ_B, with a percentage α of material A, the total density ρ_{Total} can be calculated as:

$$\rho_{Total} = \alpha\rho_A + (1-\alpha)\rho_B$$

This can be used for design purposes to selected the desired density of a composite material. Other material properties, such as elastic modulus, also continuously vary over the range of percentages, but non-linear effects and interactions between tiles make an analytical solution impractical for random halftoning. The results of simulated tensile tests of the full range of percentages varying between acrylic and aluminum are shown in Figure 6. The elastic modulus varies exponentially between the two materials. Since the halftoning is carried out randomly, 50 tensile tests were run for each material percentage, giving an approximation of the variation.

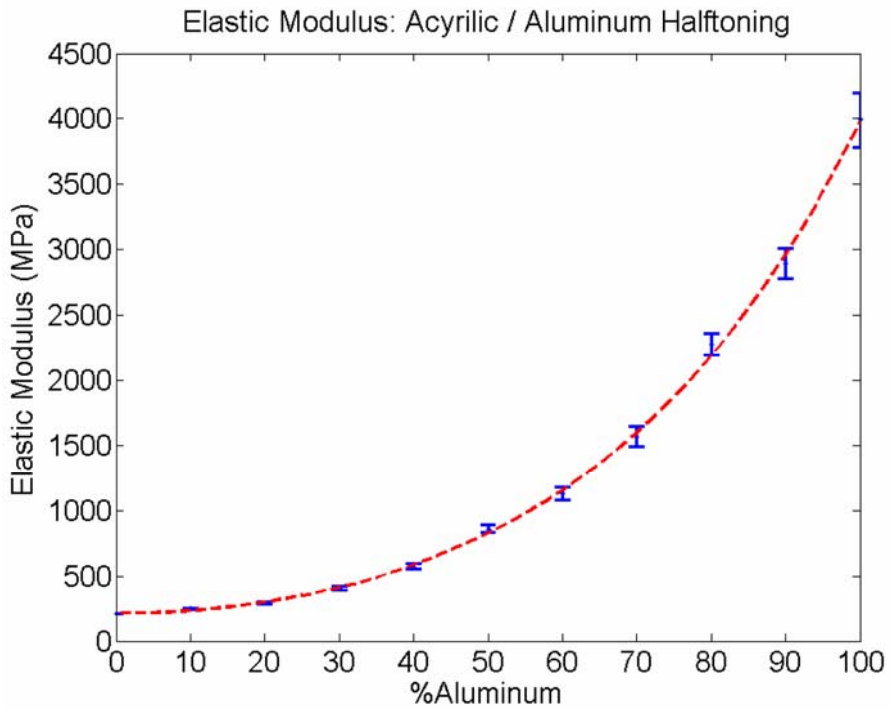


Figure 6: The elastic modulus of two-material digital structures varies continuously (in this case, with exponential fit) between the respective materials' properties (acrylic to the left and aluminum to the right) as the ratio of half-toning is varied.

In addition to tensile tests, thermal expansion tests were carried out to demonstrate the tunable CTE (coefficient of thermal expansion) of digital materials. In the same manner as density and elastic modulus, the CTE of a material may be tuned anywhere between the two aggregate materials, depending on their relative volume fractions. This is particularly interesting when one of the materials has a negative CTE (expands upon cooling) Although not common, these materials exists both in nature and in select engineering materials. One of the most common of the latter is Zirconium Tungstate ($Zr(WO_4)_2$), (Sleight, 1998) a ceramic that exhibits this property over a wide range of temperatures. The dimension of hybrid structures of Zirconium Tungstate and aluminum over a range of temperatures is shown in Figure 7. In this case, a combination of approximately 17% aluminum and 85% $Zr(WO_4)_2$ yields virtually no thermal expansion or contraction.

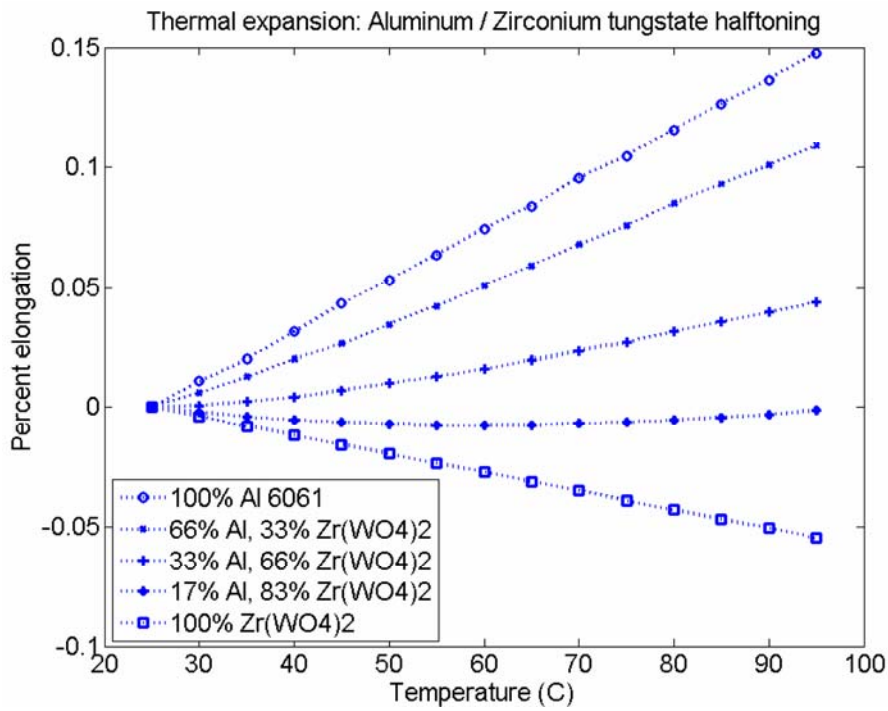


Figure 7: The thermal expansion/contraction of a digital structure made of different ratios of aluminum and zirconium tungstate demonstrates the ability to choose the desired CTE based on the percentage of each material.

Microstructure

The use of a single material or random half-tone blending yields approximately isotropic material properties in the horizontal directions of digital material composed of the square tile design. In some cases, it is desirable to introduce more anisotropy to optimize material properties in specific directions. To address this, we introduce the idea of microstructure on a voxel level. By defining a voxel sub-structure that encompasses certain properties, this "super voxel" can be tiled throughout a structure, creating a hierarchical material that reflects the properties of the sub-structure. One of the most obvious applications of this is to tune the stiffness of a hybrid material in specific direction. This can be accomplished by aligning the stiffer voxels in lines along the direction of elongation to stiffen the material.

The stiffness of a tensile specimen of various 2×2×2 microstructures is compared to the random half-toning case in Figure 8. In all cases, 50% of the voxels are aluminum and 50% are acrylic. In these tests, the tensile specimen consisted of greater than 2000 voxels, in order to ensure observation of bulk material behavior and avoid direct effects of the microstructure. Of the microstructures presented here, random, mesh, layers, and dither are pseudo-isotropic in X and Y, whereas longitudinal and transverse are at the extreme of anisotropy.

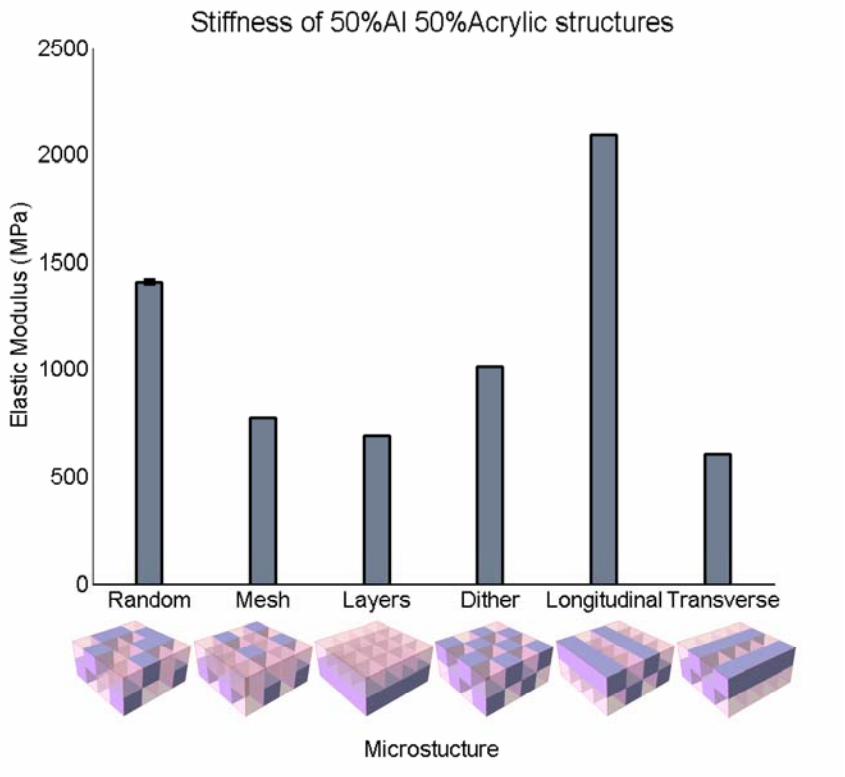


Figure 8: The properties of multi-material digital matter depend heavily on the voxel microstructure. Here, stiffness varies by over a factor of three for the same volume fraction of aluminum/acrylic

From these tests, it is apparent that the properties of composite digital materials depend heavily on the microstructure. Even selecting from only the pseudo-isotropic structures, the stiffness of the material varies by nearly a factor of two. The difference in stiffness in the extreme anisotropy case is greater than a factor of 3 in the X/Y directions. This provides yet another aspect of control over the physical properties of digital materials which could, for instance, be used to tune the stiffness of a material while keeping the density constant.

The idea of voxel microstructure may be extended to yield even more interesting properties of digital materials. For instance, auxetic materials (negative poisson's ratio) can be created. This special class of materials expands laterally when extended axially, and is useful in a wide variety of applications due to its high energy absorption and fracture resistance. (Evans and Alderson, 2000) Most auxetic materials that have been created are low density and based on foam (Lakes, 1987) or honeycomb structures, including polymer and metallic foams (Friis, 1988). Using digital material, we demonstrate in simulation a dense auxetic material made of aluminum and acrylic voxels, exhibiting a specific microstructure (Evans, 1989) of aluminum within acrylic. In theory, any combination of stiff and flexible materials would work. Using a 6×8×2 voxel base unit consisting of 68% aluminum, 48% acrylic, and only 8% voids (although the voids could be reduced further), a poisson's ratio of -0.63 was attained.(Figure 9) A similar structure with the same mass-fraction of materials and voids randomly distributed had a poison's ration of 0.11. Because the material is highly non-linear, instantaneous poison's ratio was used and plotted as a function of strain. (Smith, *et al*, 1999)

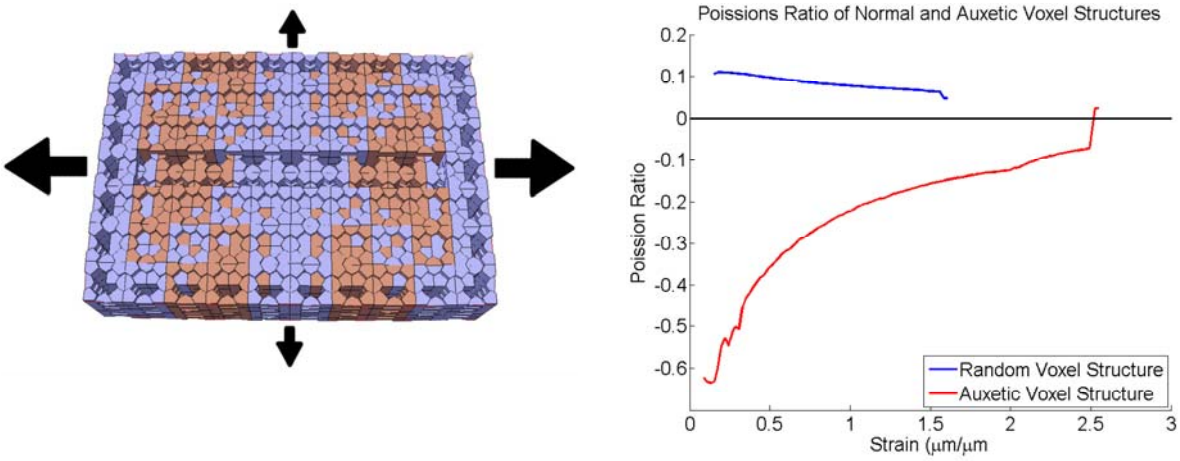


Figure 9: Digital material with a negative poisson's ratio can be created by tiling the structure shown at left. The resulting poisson's ratio as a function of strain is shown at right for material using both this structure and material with the same volume fractions of material ordered randomly.

The results clearly show the effect of the auxetic voxel microstructure. The poisson's ratio of the random pattern of voxels drops off only slightly from 0.11 until failure. However, the poisson's ratio of the auxetic microstructure increases rapidly as the

strain increases. This highlights the fact that the material does not expand linearly. However, this behavior is consistent with similar plots of previously created auxetic materials. (Lakes, 1987)

Conclusions

We have demonstrated in simulation the basis of tunable materials properties of digital materials. A wide range of density, stiffness, CTE, and failure modes may be obtained by varying voxel manufacturing precision, the percentage of randomly distributed materials, and the voxel microstructure. By varying only the precision of voxels, the stiffness and failure mode of a single material structure can be controlled. By introducing a second material and randomly half-toning a percentage of voxels between them, the material properties may be tuned anywhere between the respective properties of the two materials. Additionally, the inclusion of hierarchical voxel substructures (microstructure) allows further tuning of properties such as stiffness, and allows novel behavior such as negative poison's ratio to be obtained with dense combinations of common materials.

Based on these results, we expect digital materials to provide unprecedented control over all aspects of a bulk material. The results of these simulations are in the process being verified in physical experiments. Although only mechanical stresses displacements were output for these simulation results, the multiphysics nature of our COMSOL finite element model allows for the inclusion of friction, heat transfer, fluid flow, etc. between voxels in the finite element model for future verification. In addition, the use of 3 or more materials will facilitate the tuning of multiple material properties simultaneously.

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