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Computer-Aided Design and Manufacturing Feasibility of a
Large-Scale Collagen Protein Model for Educational Use

by

Andrew Kutas

Submitted to the Department of Mechanical Engineering
In Partial Fulfillment of the
Requirements for the Degree of

Bachelor of Science

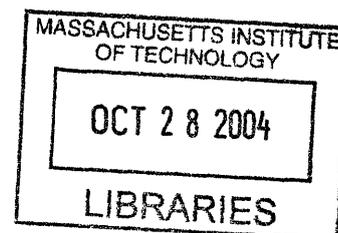
at the

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May 7, 2004

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ARCHIVES

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ABSTRACT

A collagen molecule was chosen to be manufactured for use in classroom setting. The collagen model was modeled with the SolidWorks and Catia software packages. One chain of space-filled Collagen 1CGD was modeled with SolidWorks, and the entirety of space-filled Collagen 1BKV and 1CGD was modeled with Catia. The feasibility of manufacturing the model with rigid molds was examined, and it was shown that this strategy is infeasible. One chain of ball-and-stick Collagen 1CGD was begun.

This thesis details the steps in creating the computer models and determining the manufacturing feasibility of the collagen physical model.

Thesis Supervisor: David Gossard

Title: Professor of Mechanical Engineering

Acknowledgements

I would like to thank Professor David Gossard for pioneering this project and offering me the chance to be a part of it. His guidance, both in the scope of this thesis and outside of it, has always been valuable and appreciated.

Many thanks also go to my colleague Emily Cofer, who took my work to the next step and fabricated the physical models. Without her, this project would not have reached the progress it did.

Additional thanks go to Heather Doering and Jane Yoon for their participation in this project throughout the last year.

Finally, I would like to send a warm thank you to Soraya, who always inspires the best in me.

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Chapter 1

Introduction

Protein molecules, collectively the basis for organic life, are vital parts of the study of biology. There are endless varieties of proteins, and they can be so large and complex that trying to understand the basic mechanisms can be daunting. Indeed, it can be difficult to simply visualize a large, spiraling, folding polypeptide chain.

There are currently several technologies devoted to the visualization of proteins. Online databanks exist that store coordinate information for the atoms of particular proteins and other molecules. One can use software programs to render these coordinates into electronic visualizations. Different aspects of the protein can be focused on as well: the geometric shape, the bonds, or the curling pattern can be visualized, for example.

Nevertheless, in a larger classroom setting, even this technology is not always sufficient. The experience of manipulating a computer model, while informative, is lacking compared to holding and touching the real thing. Of course, protein molecules are sized on the atomic scale and impossible for us to see and manipulate with our bare hands. Therefore, a three-dimensional physical model of a protein could serve to provide students with a learning experience that might surpass a computer model's impact.

Collagen, detailed in Section 2.1, is a good choice for a protein because its components have a relatively simple, symmetrical structure with respect to each other. Students holding a model of collagen in their hands could learn about the shape, molecular patterns, and self-interaction of the protein.

Therefore, the overall scope of the combined efforts of this thesis and that of my colleague Emily Cofer is to design and produce a physical model of the collagen protein for use in a teaching environment. This thesis is confined to the computer design of the protein, as well as using a computer model to determine which manufacturing techniques are feasible. In the following chapters, the collagen protein as well as visualization options will be discussed. Computer modeling programs and various manufacturing techniques will be touched upon. A very detailed set of instructions on how the computer files were made will be explained, with enough detail for one to be able to completely recreate the design experience. A study on the feasibility of using a rigid mold to cast the protein model will be performed using the computer models created. Finally, conclusions about the design process and future recommendations for the project will be considered.

Chapter 2

Background

Chapter 2 provides information on the various aspects of this thesis. It is important to be knowledgeable of the nature of collagen as well as different ways of visualizing the protein. Likewise, an awareness of different computer modeling and physical model manufacturing techniques is important to understand the experimentation and work that went into this project.

2.1 Collagen Protein

Collagen is a very abundant protein in the bodies of animals. Comprising 25% of all protein in humans, it provides our bodies with structural support [1]. Specifically, its great tensile strength makes it a good fit for being the primary component of ligaments and tendons [2]. It makes up 75% of human skin, and it plays a vital role in the regeneration of damaged body tissue [3].

A complete collagen polypeptide consists of three helices that wrap around each other. Figure 1 shows a partial representation of the triple helix. Then within each helix, there are primarily three different repeating amino acid units: glycine (GLY), proline (PRO), and hydroxyproline (HYP) [2]. This pattern repeats throughout the collagen chain, with some exceptions. The three-letter standard abbreviations of these amino acids are listed after the name.

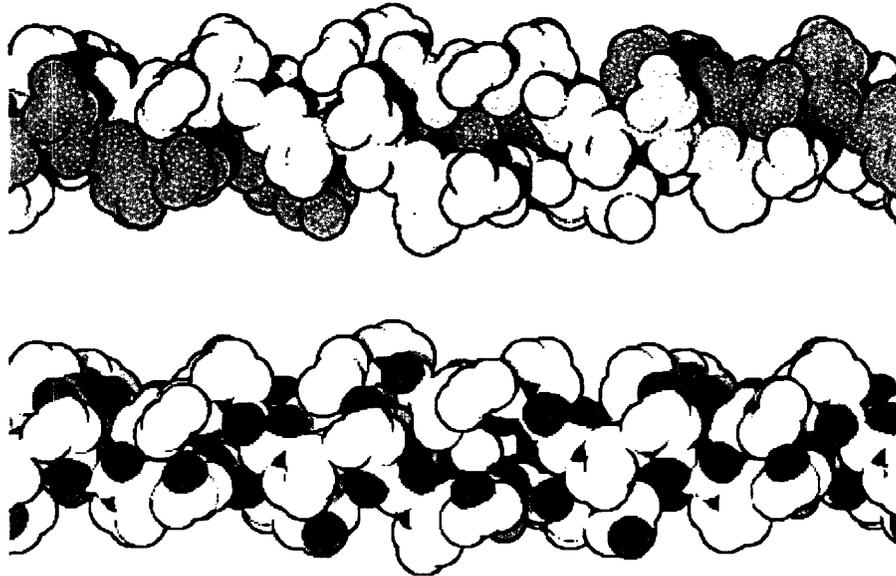


Figure 1: Partial collagen triple helix representation. Two collagen polypeptides are pictured; the top one assigns each helix a unique color. [1]

There are a variety of different collagen configurations, each with different variations in the repeating pattern. Two of these configurations are Collagen 1BKV and Collagen 1CGD. The former contains several nonstandard amino groups in the middle of the chain: isoleucine (ISO), threonine (THR), alanine (ALA), arginine (ARG), and leucine (LEU), breaking the pattern considerably. However, Collagen 1CGD only breaks the pattern once, with an alanine residue replacing one glycine residue.

2.2 Protein Visualization

A very popular resource used to visualize proteins like collagen is the RCSB Protein Data Bank (PDB) [www.pdb.org]. The PDB contains spreadsheets for many proteins that list spatial coordinates for every atom in the molecule. The

names “1BKV” and “1CGD” are actually PDB IDs that identify the two collagen variations.

The PDB also stores a list of various software that can be used to visualize proteins and other molecules. This list can be found on the PDB website at [<http://www.rcsb.org/pdb/software-list.html>]. More important than the actual visualization tools, however, are the visualization alternatives themselves. Two popular visualization alternatives are called “space-filled” and “ball-and-stick.” A space-filled model shows the complete geometry of the atoms, but it cannot show a detailed view of which atoms bond to each other. The ball-and-stick model does not preserve the actual atomic radii, but it shows which atoms are bonded to one another. Figure 2 shows a space-filled model, while Figure 3 shows a ball-and-stick model.

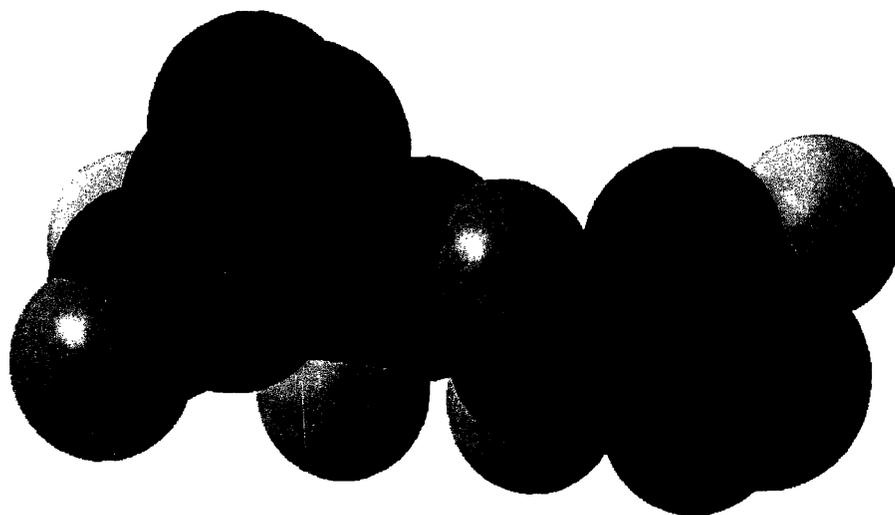


Figure 2: Space-filled model. Each sphere represents an atom, and their radii are sized in proportion to the actual molecule.

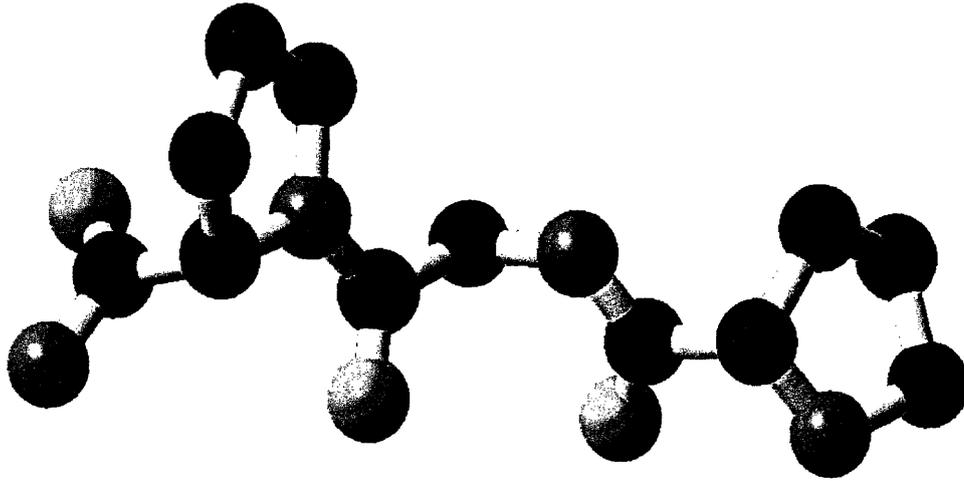


Figure 3: Ball-and-stick model. Each “ball” represents an atom, and each “stick” represents an atomic bond.

2.3 Solid Modeling Programs

There are a number of computer modeling programs available, each with its specialties and weaknesses. Two computer design suites available on MIT Windows Athena stations are SolidWorks Education Edition 2003–2004 and Catia V5, each a product of Dassault Systemes. They have slightly different user interfaces, and their relative merits are detailed in Chapter 3.

A solid modeling computer program allows for the design of a part in an electronic setting. As such, the end product of a solid modeling program is a computer file. There are a number of standard electronic formats that manufacturing sites can use to fabricate designs. Both SolidWorks and Catia have their own specific format, but they are able to convert files into more general formats. One of these popular, general formats is called STL. STL stands for “stereolithography,” [4] which is discussed briefly in Section 2.4. An STL file consists of a myriad of triangular surfaces that define the outer surface of the solid model. The smaller the triangles, the smoother the overall surface, but the

more information the STL file holds. A complex geometrical shape like a collagen molecule can result in an STL file larger than 50 MB.

2.4 Manufacture Techniques

Many different manufacturing techniques exist once the design phase of a part is complete. Usually, the more complex a design is, the more complex its manufacturing technique. Also, different techniques are sometimes better suited for different purposes. For example, a mill and lathe work well with aluminum and can create detailed features, but these machines are not optimal for mass production. Molding and casting techniques allow for faster production of parts, but because these processes are more automated, they can be limited in the geometry they are able to produce.

Collagen has a very complex geometry; therefore, the more conventional manufacture techniques are not feasible. For instance, it would be possible but painstakingly difficult and time-consuming to use a computer-automated mill to produce a collagen physical model. A better strategy would be to combine the versatility of rapid prototyping with the repeatability of casting parts from molds.

Rapid prototyping is often conceptualized as “three-dimensional printing” [5]. There are several techniques with rapid prototyping that quickly produce a three-dimensional part. The first technique to be invented was stereolithography, and it works by starting with an STL file, slicing it into very thin layers, and constructing the slices one layer at a time [5]. These layers consist of liquid photosensitive polymers that, when exposed to ultraviolet, become solid [5]. A newer technique, invented at the Massachusetts Institute of Technology, is Three

Dimensional Printing. This technology also constructs physical parts as an aggregation of slices. Instead of using photosensitive polymers, though, it uses any material that can be made into powder form, and it combines the slices with a binding substance [6].

Different molding and casting techniques are also available. The main issue for complex shape like collagen is if it can be cast in a rigid mold. As Chapter 4 details, a rigid mold has limitations on how the part can be separated from it. A flexible mold might be necessary due to the many contours of the part. One technique that can produce a flexible mold is Room Temperature Vulcanization. This process yields a flexible silicone mold that can be used to cast a small number of parts [7]. The molds retain detail well and accommodate a large variety of part materials [7].

Chapter 3

Space-filled Collagen Model

Both SolidWorks and Catia were used to make computer models of a collagen protein. While SolidWorks is a useful and very capable solid modeling package, its user interface was cumbersome and not as well-suited as Catia for three-dimensional object creation. Catia provided better flexibility and more intuitive controls for creating and placing features in three-dimensional space. Therefore, SolidWorks was abandoned for Catia as the software package of choice for the creation of solid models.

One should note that in the creation of the space-filled models, the absolute dimensions are not important, so long as the same unit of measure is used consistently in a given model or set of models. The STL files carry the dimensions, but they can be scaled to fit the constraints of the manufacturing process that will make a physical model from the file.

3.1 SolidWorks Approach

In SolidWorks it is inconvenient to make a model like Collagen 1CGD in the SolidWorks Part domain. The solid model comprises a collection of spheres, each representing an atom, and each with its own 3D-space coordinates. To create a point with arbitrary 3D-space coordinates in a SolidWorks Part file, one can use the **3D Sketch** command from the **Insert** menu. However, to create a sphere centered at this point, one must first create a plane containing the point, then create a sketch of a semicircle whose diameter intersects the point, and finally

revolve this semicircle about the diameter. As such, it is more convenient to work in a SolidWorks Assembly file. One can create Part files for each atom, then insert them into the Assembly file at desired points.

A spreadsheet of coordinates for Collagen 1CGD, available online at [<http://www.pbd.org>], was used to determine the coordinates and radii of the atoms making up the protein. Only one chain, Chain A, was made. First, the individual atoms were created as SolidWorks Parts. Starting with the carbon atom Part file, the **Front** plane was selected. A sketch was created on this plane by selecting the **Sketch** command in the **Insert** menu. Using the **Circle** tool from the **Sketch Tools** palette, a circle was created with its center on the origin. Its radius was set to 1.7 in. Then, the **Centerline** tool from the **Sketch Tools** palette was used to create a diameter of this circle. The cursor was placed near the top of the circle and it hovered around the area until it located the point that coincided with the circle and was completely vertically above the origin. After selecting this as the starting point of the line, the second point was created at the bottom of the circle, also using the technique of hovering until the point was automatically located. If these automatic constraints are not available, one must create the centerline and later add the vertical and coincident constraints to it. Then, the **Sketch Trim** tool from the **Sketch Tools** palette was selected, and the circle was clicked on the right side of the sketched vertical diameter. This operation left a semicircle as shown in Figure 4.

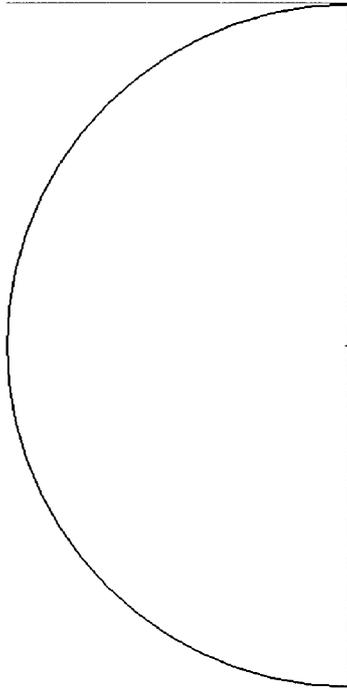


Figure 4: Semicircle. The semicircle will be revolved about the centerline to produce a sphere.

Afterwards, the **Revolve...** command was selected from the **Surface** submenu in the **Insert** menu, and the semicircle was selected. The revolve parameters were **One-Direction** and **360deg**. This created a sphere with radius 1.7.

Finally, the sphere was right-clicked and **Face Properties** was selected. The color was changed to black (Red 50 Green 50 Blue 50), resulting in a sphere as shown in Figure 5. In the same fashion, spheres representing oxygen and nitrogen were created with radius 1.4 and 1.5, respectively. Their colors were red (Red 255 Green 50 Blue 50) and blue (Red 0 Green 128 Blue 255), respectively.

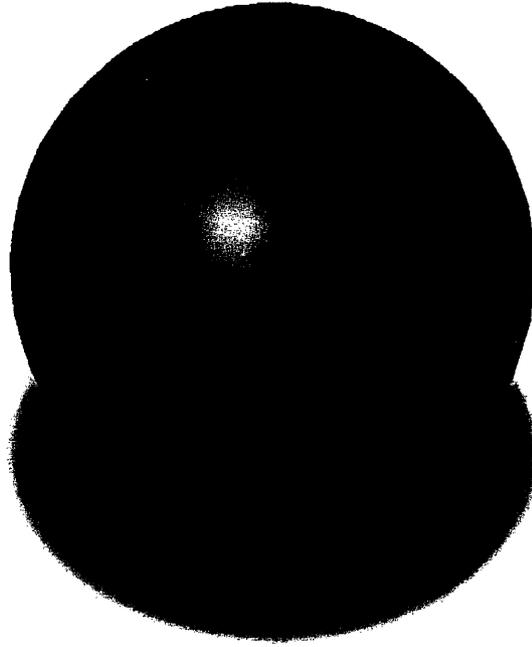


Figure 5: Carbon atom. This black sphere will represent carbon in the collagen model. Oxygen and nitrogen will be represented by red and blue spheres, respectively.

The next step was to incorporate these spheres into an Assembly file, representing the aggregation of atoms into one large molecule. A new Assembly file was created, and each atom file was opened. To make each atom in the molecule, the sphere of the appropriate type was dragged from its Part window into the Assembly window. Then, the sphere was selected and **Move Component** from the **Assembly** palette was selected. In the **Move** box, pictured in Figure 6, the **To XYZ Position** was selected. The atom's coordinates were entered here. This process was repeated for each atom in Chain A until the final molecule was created, which Figure 7 shows.

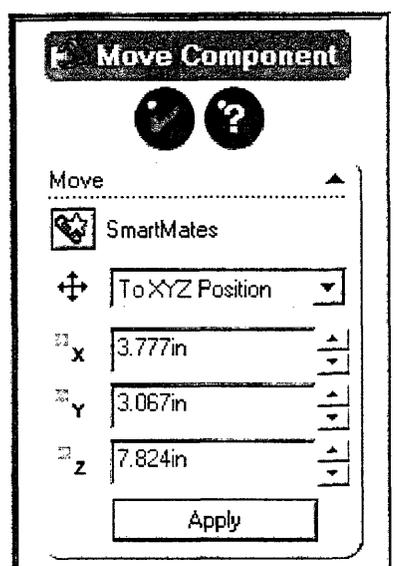


Figure 6: Move Component box. The To XYZ Position selection was manually chosen from its pull-down window. Then, the coordinates could be entered.

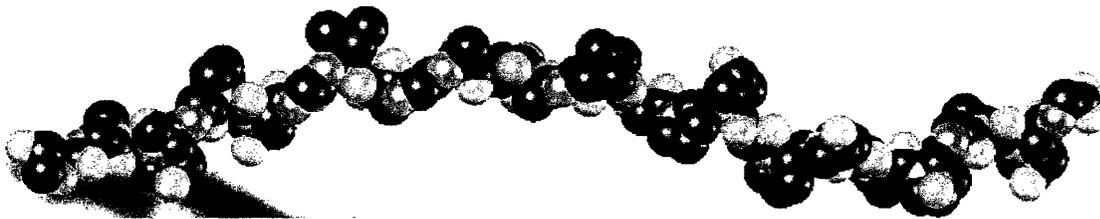


Figure 7: Final Collagen 1CGD Chain A model. The complete chain contains 192 atoms.

The file was saved first as a SolidWorks Assembly file. Then, it was converted into an STL file by choosing **Save As...** from the **File** menu and selecting **STL (*.stl)** as the file type.

3.2 Catia Approach

In Catia it is simple to work in 3D-space in the Part domain. Two sets of three chains were created: Collagen 1BKV and Collagen 1CGD. The Catia user interface is also flexible enough to allow easy editing and reconfiguration of parts

in 3D-space. Therefore, a template model was made for Collagen 1BKV Chain A, and models of the other chains were produced by editing this first chain.

3.2.1 1BKV

Catia was launched. As Figure 8 shows, from the **Start** menu and **Mechanical Design** submenu, the **Part Design** domain was selected.

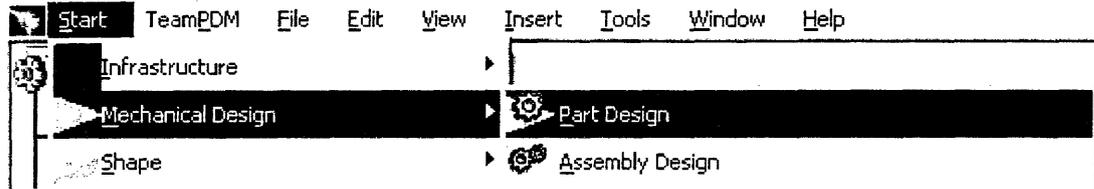


Figure 8: Part Design location. Catia features many design interfaces, so it was important to choose a proper environment for making the design.

Before creating the geometry of the model, a custom tool palette was created. The **Customize...** subcommand was chosen from the **Toolbars** command in the **View** menu. A new toolbar was created by clicking the **New...** button. The new toolbar, **NewToolBar001**, was selected in the menu, and the **Add commands...** button was clicked. Figure 9 shows the **Customize** window and the location of **NewToolBar001**.

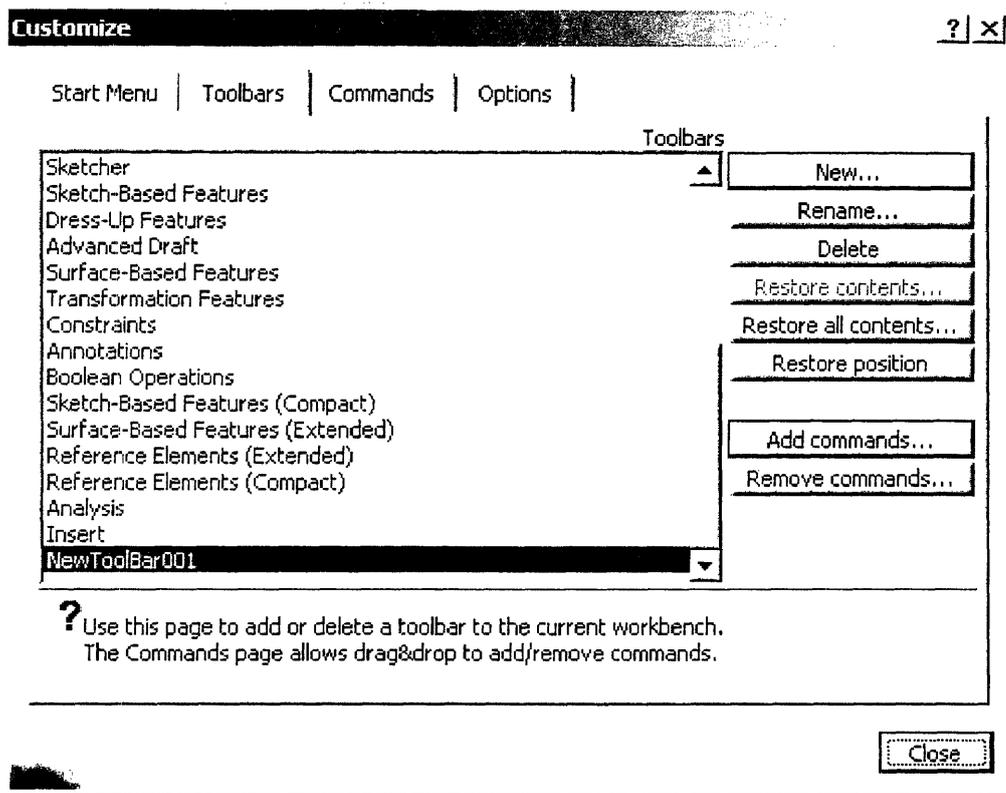


Figure 9: Customize window. A custom toolbar palette was created here.

The **Point...** and **Sphere...** commands were selected in the **Commands list** window, pictured in Figure 10, by holding the Ctrl key and clicking, then the **OK** button was clicked.

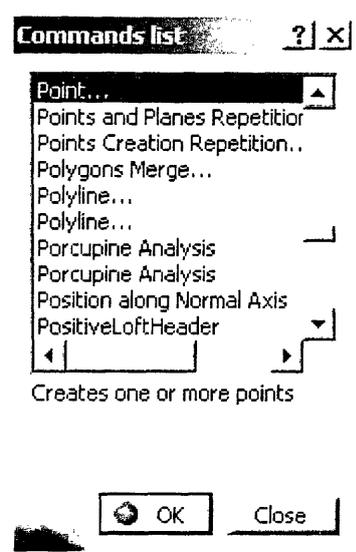


Figure 10: Commands list window. The **Point...** and **Sphere...** commands were chosen from this window.

Then, the **Point...** command was selected, and the coordinates for the first atom were input into the **Point Definition** dialog box, making sure **Coordinates** was selected as the point type, and **Default (Origin)** was selected as the Reference, as Figure 11 shows. The Collagen-1BKV coordinates, also available at online, list the coordinates of the first atom as pictured in Figure 11.

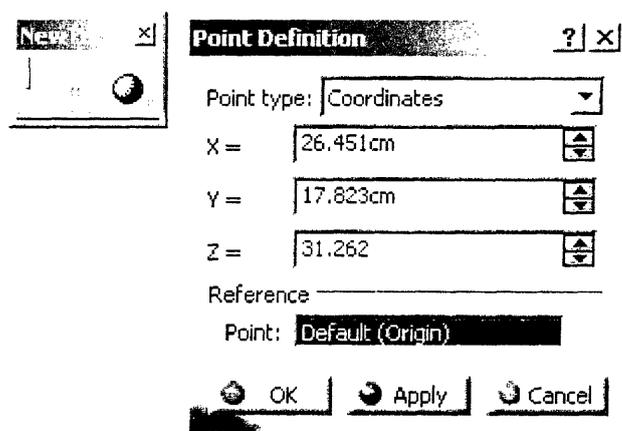


Figure 11: NewToolBar001 and Point Definition windows. The orange square is the clicked appearance of the **Point...** tool.

To make the sphere, the newly created point **Point.1** was selected and the **Sphere...** command was chosen from the custom tool palette. The corresponding atomic radius—in this case, 1.4 for nitrogen—was input in the **Sphere radius** field. The sphere icon was selected as shown in Figure 12 so that a full sphere instead of a partial spherical surface would be made.

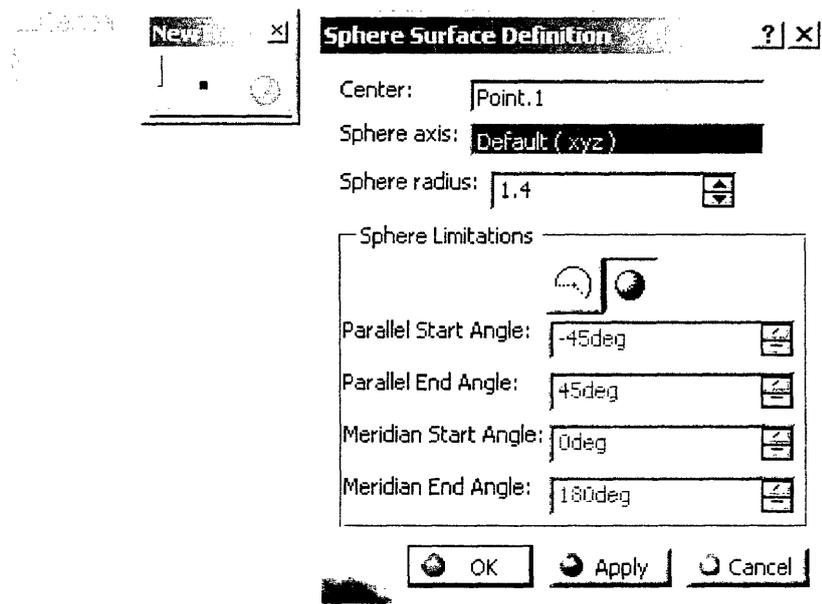


Figure 12: Sphere Surface Definition window. The red X labeled **Center** is **Point.1**. The orange sphere represents the clicked appearance of the **Sphere...** command.

Then the **OK** button was clicked.

This process was repeated for the remaining 183 atoms in Collagen 1BKV Chain A, resulting in the complete molecule pictured in Figure 13.



Figure 13: Collagen 1BKV. Note the protruding residue in the middle of the protein. This is a tell-tale signature of Collagen 1BKV.

The model was saved as a Catia Part file, the default setting. Then, it was converted into an STL file by selecting **Save As...** in the **File** menu, then selecting **stl** as the Save as type.

To make the other two chains, it was not necessary to start this process all over again. Instead, because the order of the atoms in each chain is mostly identical, only the location of the points needed to be changed. Each sphere was linked to a parent point, so when the point moved, the sphere followed it. The only difference between Chain A and Chains B and C in terms of atomic makeup is that Chain A lacks the first residue, proline. Therefore, seven additional points and spheres had to be created to include this residue, using the process detailed in this section. For the rest of the points, each was double clicked in the Tree, and its coordinates were changed to the corresponding value of the Chain B, as Figure 14 shows.

Figure 15 shows the completed Chain B computer model. It too was saved as a Catia Part and an STL file. Afterwards, the point coordinates were changed to match those for Chain C, and the model was saved and converted.

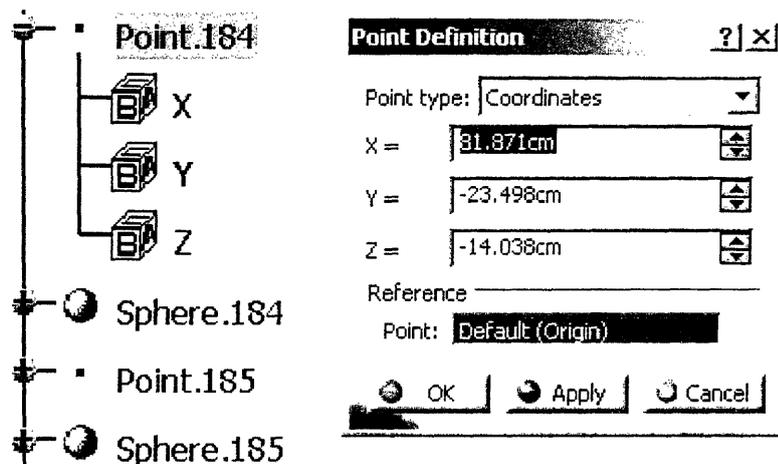


Figure 14: Changing the point coordinates. Point.184 was highlighted in the Tree, and the new coordinates were entered.



Figure 15: Collagen 1BKV Chain B. This chain looks very similar to Chain A, except it has the first residue. Chain A does not have information for its first residue.

3.2.2 1CGD

After the Collagen 1BKV chains were made, it was decided that Collagen 1CGD, which breaks the repeating residue pattern only once, would be a better model to produce. All three chains were to be modeled. The two proteins have a very similar atomic pattern at the beginning and the end of each chain. However, at atom #64, the two versions diverge. They converge again at atom #73, but after atom#109, Collagen 1CGD has two extra atoms that Collagen 1BKV simply lacks. See Table 1 for a detailed comparison of the two versions at these atom numbers.

Table 1: A comparison of 1CGD and 1BKV from atom # 64 to #72.

Atom #	64	65	66	67	68	69	70	71	72
1CGD	CD	N	CA	C	O	CB	CG	CD	OD
1BKV	CG	CD	N	CA	C	O	CB	OG	CG

Due to the differences, a modified approach to creating Collagen 1BKV Chains B and C from Section 3.2.1 was used to create Collagen 1CGD Chain A. Up to atom #64, the same method of changing the coordinates of the points was used. At atom #65, which for 1BKV is nitrogen and for 1CGD is carbon, the point coordinates *and* the sphere radius were changed. At these locations, the sphere was double-clicked in the Tree, and its radius was changed to the appropriate size. This process was repeated for each point location in which the atoms of 1BKV and 1CGD are not the same. Two additional points and spheres were also created because Collagen 1CGD has 192 atoms per chain, while Collagen 1BKV has only 190.

After the point locations were changed, then the names of the points and their corresponding spheres were changed to reflect the proper order of the atoms according to the 1CGD coordinates available online. This was done by right-clicking each point in the Tree and selecting **Properties**. Then, the **Feature Properties** tab was selected, and the name was changed to reflect its order in the Chain, as Figure 16 illustrates.

Finally, each residue in Chain A was assigned a unique color to illustrate the periodic nature of the residues within a collagen chain. Each point and sphere of a given residue was selected, as dictated by the coordinates spreadsheet. Then, the group was right-clicked and Properties was chosen, as Figure 17 shows.

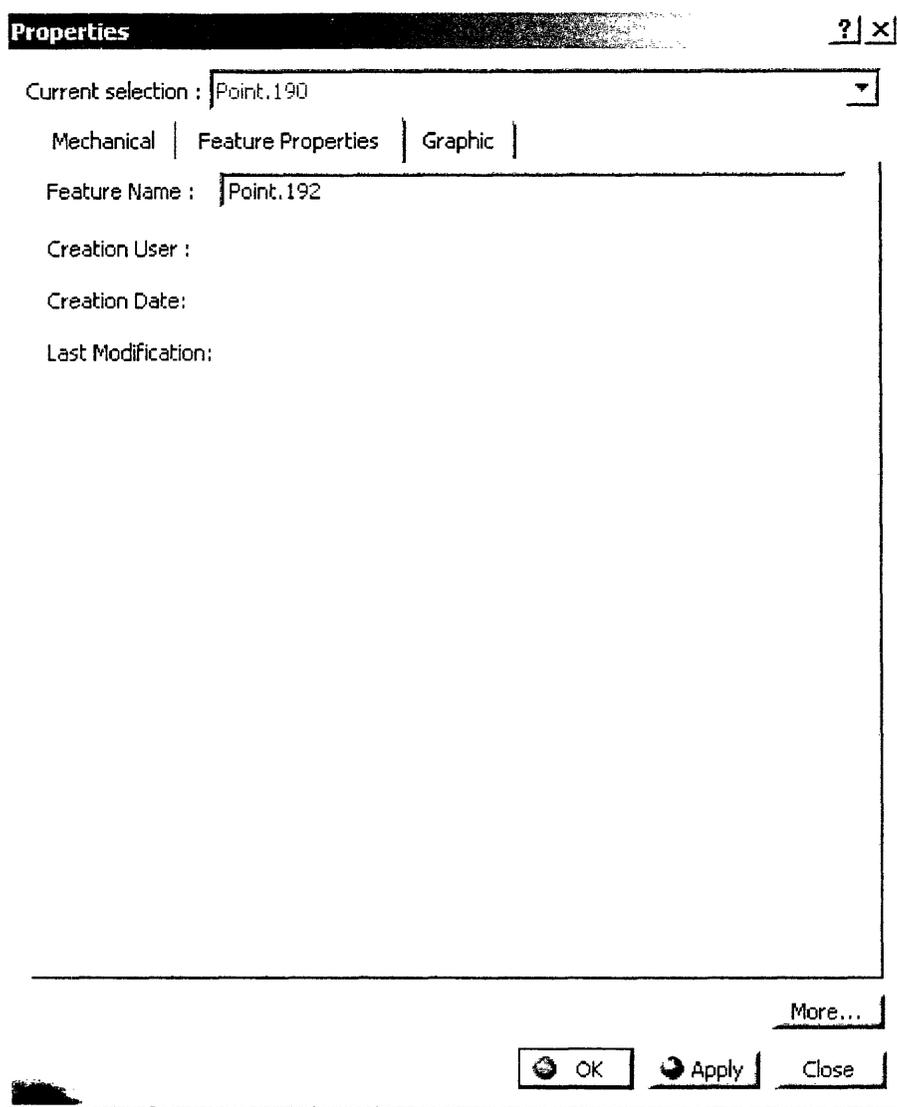


Figure 16: Properties window. The name was given a new number to reflect the proper order of the atoms.

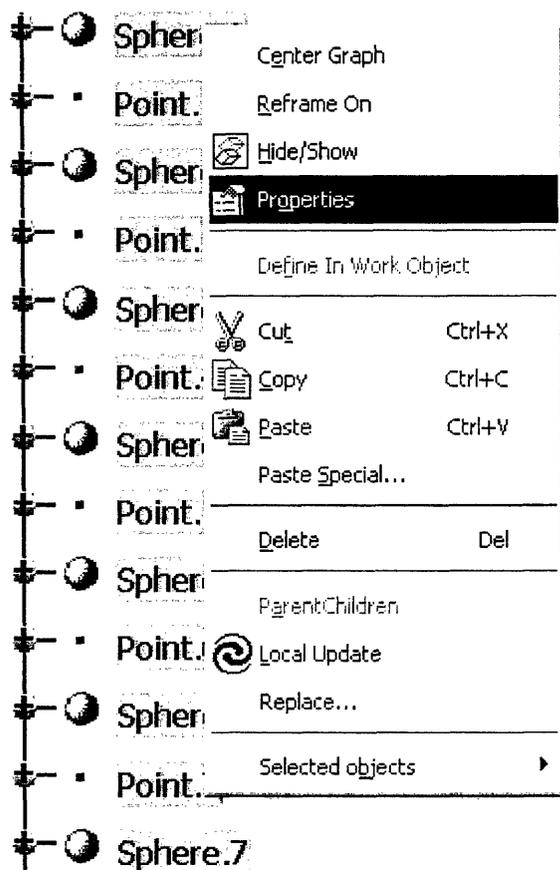


Figure 17: Selecting multiple objects. Each selected point and sphere belong to the first proline residue.

The **Graphic** tab was clicked, and **More Colors...** was selected from the Color pull-down box in the Fill section to create a set of custom colors. The **Define Custom Colors** button was clicked, and a dark red was chosen (Red 127 Green 0 Blue 0). A blank square in the **Custom Colors** palette was selected, and the **Add to Custom Colors** button was clicked. The same was done for dark blue (Red 0 Green 0 Blue 127) and dark magenta (Red 127 Green 0 Blue 127). Figure 18 shows the resulting appearance of the **Color** window.

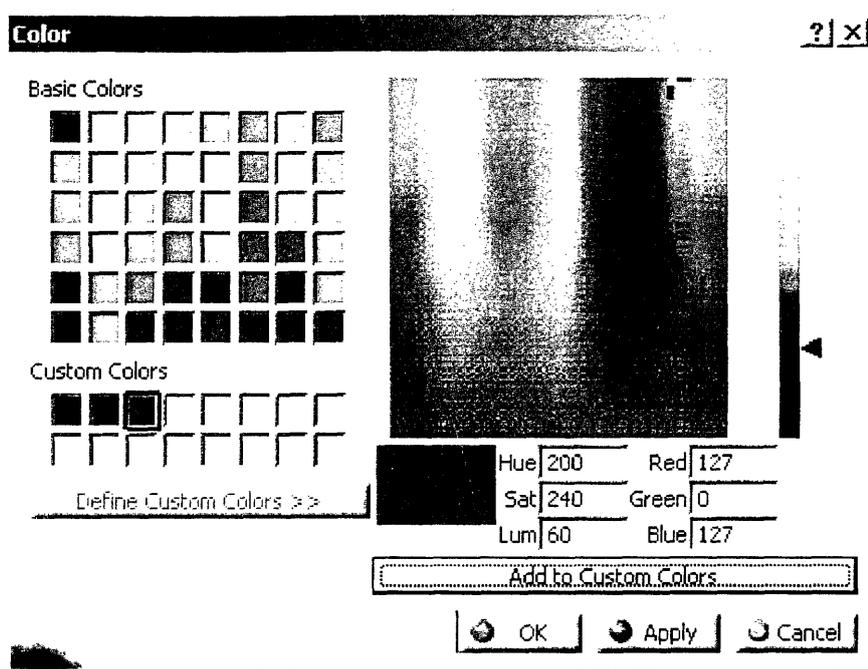


Figure 18: Color window. Custom colors were created to classify the different residues in the chain.

The **OK** button was pressed, and the dark red color was selected in the **Color** pull-down boxes in each of the **Fill**, **Edges**, and **Points** sections. Dark red corresponded to proline, dark blue to hydroxyproline, dark magenta to glycine, and black to alanine. The final Collagen 1CGD Chain A model is shown in Figure 19.



Figure 19: Collagen 1CGD Chain A. This representation shows the periodic pattern of the residue groups.

To make Chains B and C, the coordinates of each point were changed to reflect the new values using the same process as in Section 3.2.1. No other changes were necessary because the three chains in Collagen 1CGD have the same atomic pattern. The resulting computer models look practically identical to Chain A in Figure 19 above so are not included individually.

Chapter 4

Parting Line Feasibility

Both the SolidWorks and Catia approaches produced functional STL files to use in manufacturing a solid model of a collagen protein. However, there are many options available to manufacture a model, as Section 2.4 details. My colleague Emily Cofer pursued the different manufacture options and determined the proper method to fabricate a part from the computer model. My role in this investigation was to determine if a traditional parting line could be created for a hypothetical rigid mold of this model. The results of this process steered the direction of the manufacturing process selection from conventional methods, like injection molding, to more complex methods, such as room temperature vulcanization.

4.1 Criteria for Translational Motion only

Common rigid molds consist of two halves: the cavity and the core [7]. When they are put together, they leave a space. This space has the shape of the desired part. An example of a mold cross-section is pictured in Figure 20.

In the basic molding process, the mold halves are put together, the space between the molds is filled with the part's material, the part material hardens, and the mold halves are removed from the part. Of course, this explanation ignores other essential requirements of molding. Only the geometry of the molding process is relevant for determining the feasibility of incorporating a rigid-mold parting line.

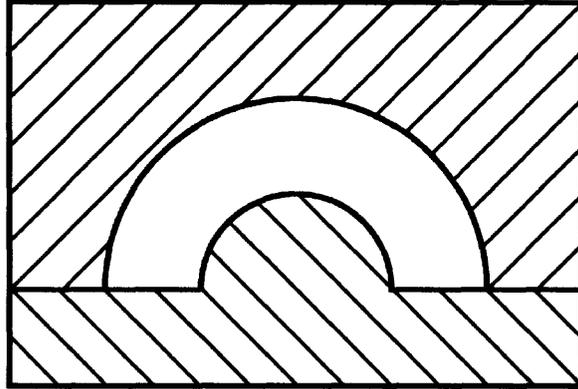


Figure 20: Mold cross-section. The space between the mold halves is the shape of the cast that will be produced in them.

Figure 21 illustrates the basic process of removing rigid mold halves. Again, many basic molding necessities are ignored; only the geometry is relevant. Also, it is assumed that the molds only undergo translational motion. Rotation of the mold, such as for a spiral, is studied in Section 4.2.

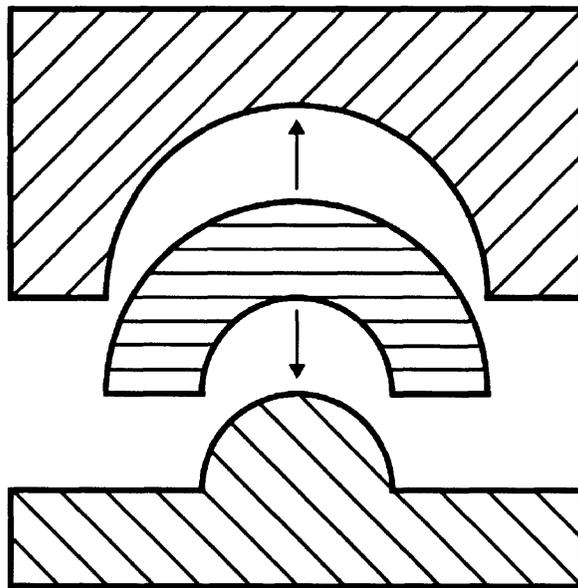


Figure 21: Removing the mold halves. There must be clearance for the mold halves to slide away from the part

The molds must translate away from the part. If the molds and the fabricated part are all rigid, then the geometry must accommodate the separation of the part from the mold. (If either the mold or the part is flexible, then it can change its shape to accommodate geometry that would otherwise prevent the separation of the two.) Figure 22 shows three mold cross-sections. The first two have geometry that accommodates the separation of rigid parts. The third cross-section, however, has a shape that prevents the separation of the part inside it.

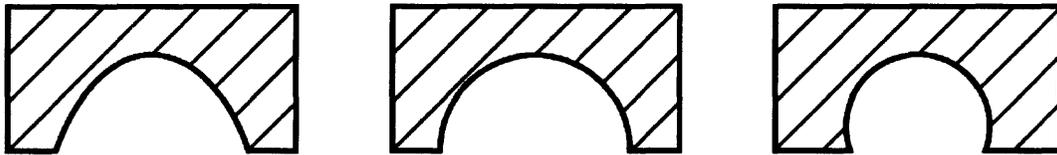


Figure 22: Mold cross-sections. The first two molds have geometry that allows the part to slide out, but the third mold has geometry that prevents the part from sliding out.

The key to successful removal of rigid parts lies in the convergence of tangent lines in the contour of the cavity. Reexamining the three example cross-sections from Figure 22 above, one can see a difference in the convergence of the tangent lines of the cavity contours. In Figure 23 below, for the first mold cross-section, the tangent lines of the cavity contour converge into the direction of the mold. For the second mold, the tangent lines are parallel and never converge. In the third mold, the tangent lines of the cavity contour converge away from the mold—that is, they diverge into the mold.

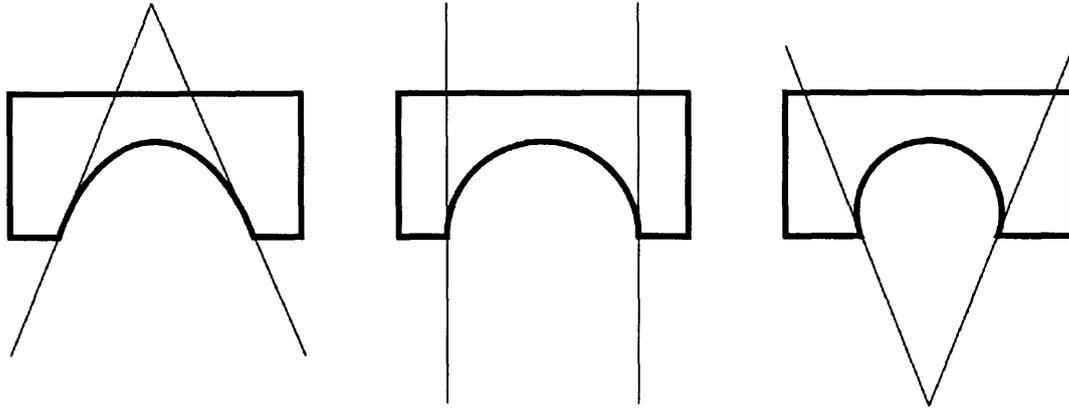


Figure 23: Convergence of tangent lines to mold contour. As long as the lines do not diverge into the direction of the mold, the cast part is able to slide out.

Also note that the contour of the mold cavity is one and the same as the contour of the cast part itself. Therefore, the criterion for successful removal of a rigid part from a rigid mold with only translational motion is that the tangent lines of the contour of the part never diverge into the mold.

4.2 Criteria for Rotational and Translational Motion

The allowance of rotational motion when separating the part from the mold yields additional part design possibilities. Primarily, screws, spirals, and other helical patterns are possible. If rotational motion is prohibited, then spiral shapes with “holes” in the middle would not be able to be removed from molds because they wrap around the mold material. They would have to be twisted out of the mold, very similar to unscrewing a screw. In this case, though, the same contour tangent line criterion applies. As Figure 24 shows, if the spiraling contour has any concave features, it will not be able to be unwound from inside the mold.

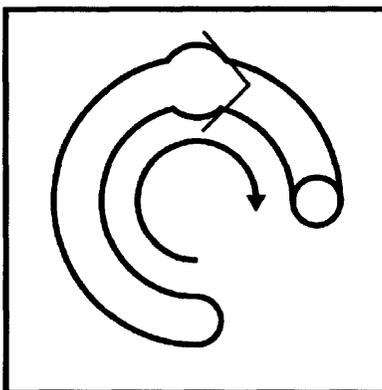


Figure 24: Cast part with helical contour. The cast part must be twisted out in the direction of the arrow. If its geometry includes a bump as shown, it will not be able to be removed. This is an extension of the converging tangent line criterion.

4.3 Parting Line Feasibility in Collagen Residue

In order to determine if a collagen chain solid model could be fabricated using rigid molds, it must be put to the tangent line divergence test described in Sections 4.1 and 4.2 above. The computer model whose creation is detailed in Section 3.2.1 above was used to examine the geometry of collagen and determine the feasibility of using a rigid mold.

If part of the collagen chain does not fit the rigid-mold parting line criteria, then the whole chain must not either. The first three residues of Collagen 1BKV Chain A were examined to test the parting line feasibility. As Figure 25 shows, each atom was assigned a unique color. This aided in identifying the orientation of the residue triplet when seen from different points of view.

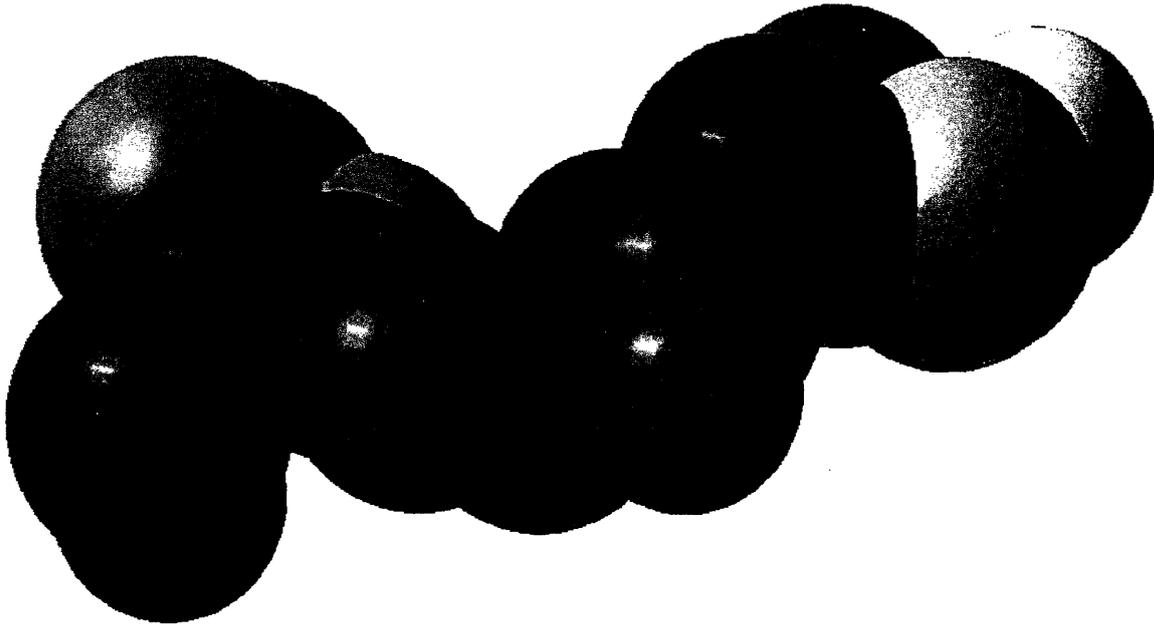


Figure 25: First residue triplet. Hydroxyproline is blue, glycine is purple, and proline is red.

The most logical direction to place a parting line would be where the part is at its most horizontal. That way, the features of the part are distributed along the surface of the mold, and there would be the least chance that the tangent line criterion fails. Figure 26 shows a simplified representation of this explanation.

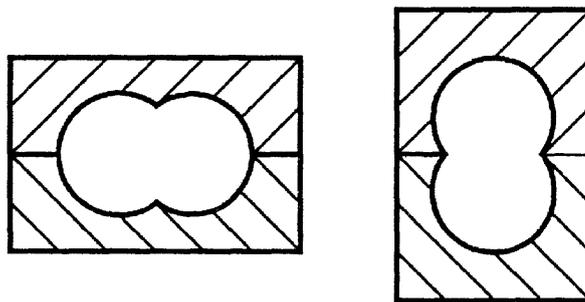


Figure 26: Horizontal vs. vertical orientation. The horizontal orientation on the left allows for a piece to be removed when the molds separate. However, the vertical orientation on the right does not allow the removal of a cast piece.

The residue triplet was examined at its most horizontal orientation. A horizontal plane was added to the triplet, separating it into top and bottom halves. The plane made it easier to visualize the angle of the tangent lines of the contour of the triplet. Figures 27 and 28 collectively show that the counter tangent line criterion fails. Every time a sphere is intersected by the plane but not through its center, it runs the risk of not fulfilling the tangent line criterion. Figure 26 above illustrates this: the first mold interfaces at a plane that intersects the two circular cross-sections through their center. However, the second mold interfaces at a plane that does not intersect the circular cross-sections in their centers.

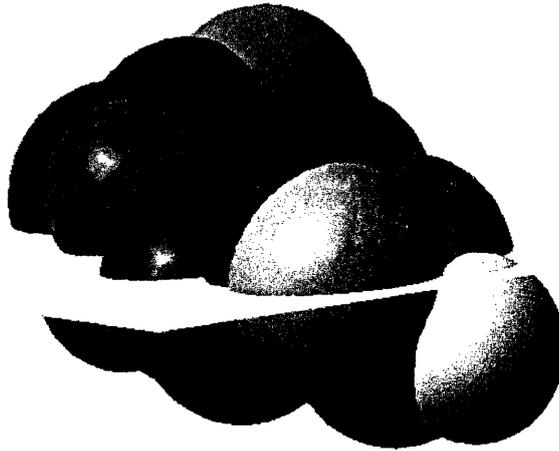


Figure 27: First residue intersected by plane, isometric view. The plane makes it easier to visualize the angles of the tangent lines to the surface counters with respect to the plane.

One can visualize that no matter the height or the orientation of the plane, at least one sphere will not be intersected through its center. Therefore, at least one pair of tangent lines will diverge into the hypothetical mold location.

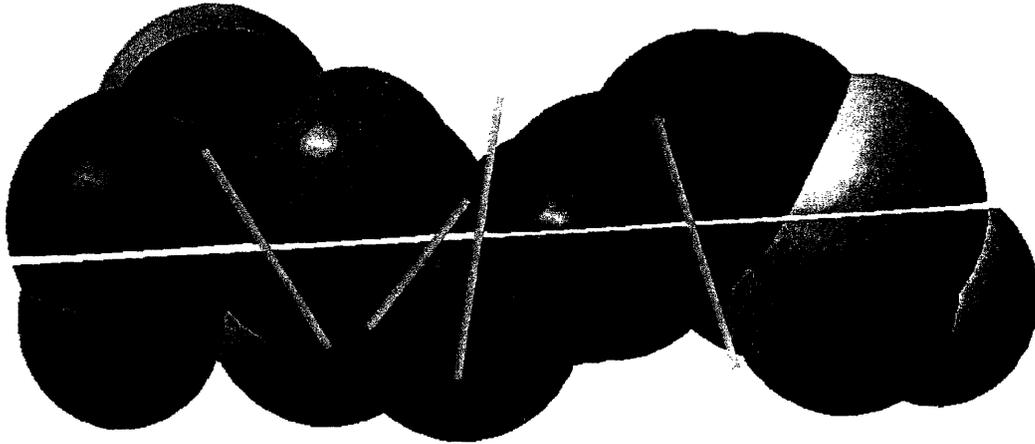


Figure 28: First residue intersected by plane, side view. The red lines show two examples of tangent lines that would diverge into the theoretical mold.

Figure 29 shows a rotated view of Collagen 1BKV. The spiral pattern is not easily observed when the model is oriented to show its length. However, this rotated view shows that collagen is a spiral shape with a “hole” in the middle. Because the helical contour also has many concave features, it fails the parting line tests described in Section 4.2.

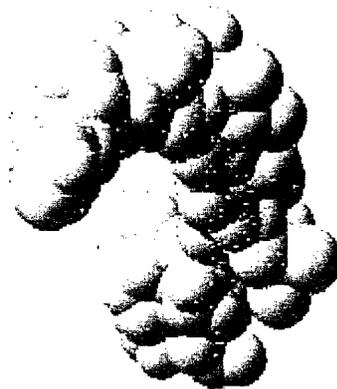


Figure 29: Spiraling nature of Collagen 1BKV. The molecule has the shape of a spiral that makes a complete revolution and has a “hole” in the middle.

And thus, it was demonstrated that the collagen model could not be manufactured using rigid molds.

Chapter 5

Ball-and-Stick Collagen Model

A computer model of ball-and-stick Collagen 1CGD A was begun. Although its progress was halted in order to make computer models of Chains B and C, it could be completed following the steps detailed below.

First, the entire model was highlighted by selecting **Open-body.1** in the Tree. Then, this selection was right-clicked, and **Hide/Show** was selected, resulting in a blank workspace for the time being.

The next step was to create new, smaller spheres to represent the atoms. For each atom, its corresponding point was selected from the Tree. Then, the **Sphere** icon from the custom palette was clicked. In the **Sphere Surface Definition** dialog box, the radius was entered as **0.5** and the full sphere icon selected. The **OK** button was clicked to make the sphere. Each point was selected, and a sphere of radius 0.5 was created in this way.

To differentiate between the types of atoms, different colors were assigned to the spheres using the same technique as described in Section 3.2.2. The same scheme as in Section 3.1 was used: black (Red 50 Green 50 Blue 50) for carbon, red (Red 255 Green 50 Blue 50) for oxygen, and blue (Red 0 Green 128 Blue 255) for nitrogen. The result for the first three residues is shown in Figure 30 below.

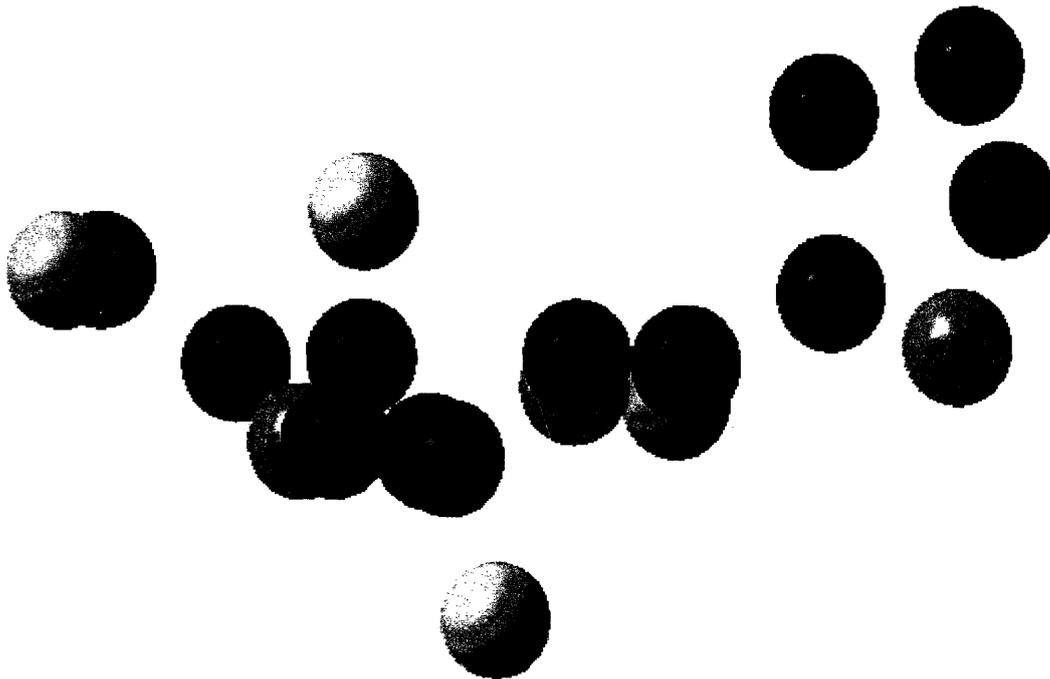


Figure 29: Isolated spheres in ball-and-stick model. These spheres represent the atoms in the first residue triplet.

In order to continue, new commands had to be added to the custom menu. The **Customize** subcommand was chosen from the **Toolbars** command in the **View** menu. The custom toolbar was selected in the **Toolbars** tab, and the **Add commands...** button was clicked. In the **Commands list** window, the selections **Circle...**, **Extrude...**, **Line...**, and **Plane...** were each control-clicked. Then, the **OK** button was clicked, and the **Close** button in the **Customize** window was clicked. The resulting custom palette is shown in Figure 30.



Figure 30: Further customized NewToolBar001 palette. The **Circle...**, **Extrude...**, **Line...**, and **Plane...** commands were just added.

While some of these commands are readily available in other menus and/or toolbars, it is more convenient to store them all in one location.

The next step was to create lines between spheres. These represented the bonds between bonded atoms. They would be used to create cylinders, which would be the “sticks” in the ball-and-stick model. The location of these lines—that is, which spheres they connected—was not trivial. An image of an outside ball-and-stick Collagen model was consulted to determine the proper line locations.

The following connection pattern was detected:

Proline: N—CA, CA—C, C—O, CA—CB, CB—CG, CG—CD, CD—N.

PRO-HYP: C(PRO)—N(HYP)

Hydroxyproline: N—CA, CA—C, C—O, CA—CB, CB—CG, CG—CD,
CG—OD, CD—N.

HYP-GLY: C(HYP)—N(GLY)

Glycine: N—CA, CA—C, C—O

GLY-PRO: C(GLY) to N(PRO)

To make a line, the **Line** icon was clicked in the custom palette. **Point-Point** was automatically selected in the **Line type** field, but if this is not the case, be sure to select **Point-Point**. Then, **No selection** in the **Point 1** field was automatically highlighted. According to the Collagen-1CGD spreadsheet, atom #1 is N in the first pro residue, and atom #2 is CA in the same residue. Therefore, **Point.1** in the Tree was clicked for the **Point 1** field. **No selection** in the **Point 2** field was now highlighted, and **Point.2** in the Tree was clicked, making the **Line Definition** window appear as shown in Figure 31. The **OK** button was clicked.

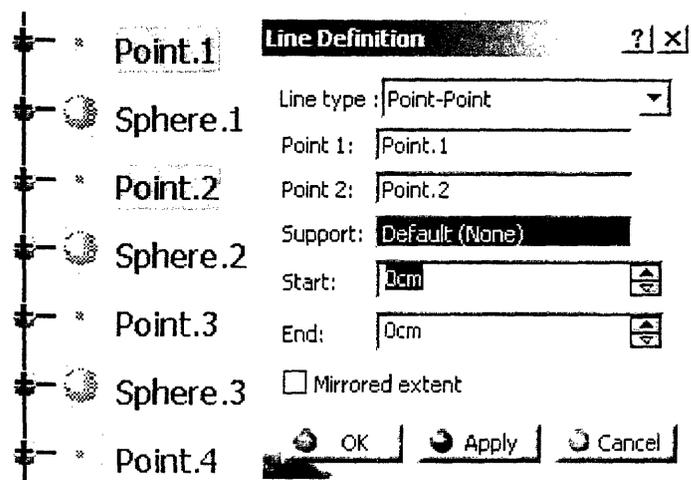


Figure 31: Line Definition window. This tool can make a line between two points.

This process was repeated for the points representing the atom pairs listed above, until they were all completed. Then in the Tree, all the **Line** items were selected, the collection was right-clicked, and **Properties** was selected. Under the **Graphic** tab, cyan was chosen in the **Color** pull-down menu in the **Lines and Curves** section. Also, in the **Thickness** pull-down menu, **2** was chosen for extra visibility. The **OK** button was clicked, and the result is shown below in Figure 32.

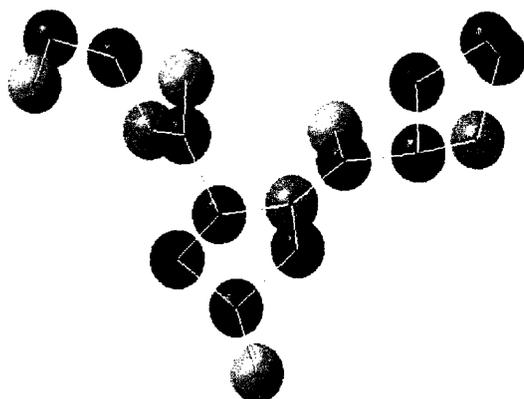


Figure 32: Spheres and lines in ball-and-stick model. Cylinders will be made, centered on each cyan line, to represent the “sticks.”

Next, for each line, a plane normal to the line and coincident with one of the endpoints was made. The **Plane...** icon was clicked from the custom palette, and Figure 33 shows the **Plane Definition** window that opened. Plane type was changed to **Normal to curve**, and **Line.7** and **Point.1** were chosen as the parameters, resulting in the green plane also pictured in Figure 33.

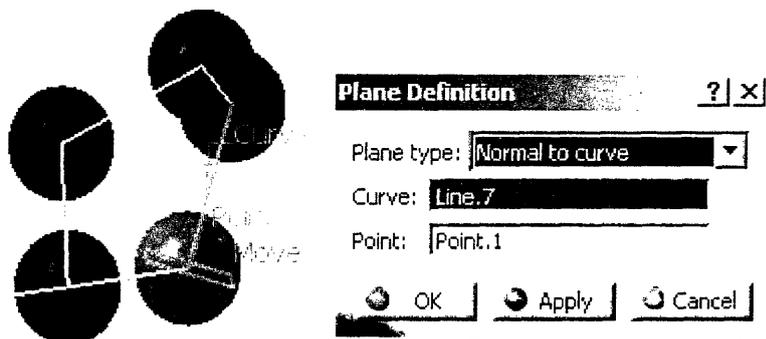


Figure 33: Plane Definition window. These parameters created the green plane coincident with the center of the blue nitrogen atom.

The **OK** button was clicked to make the plane. Planes were made for every other line in the same manner. Afterwards, circles were made on the planes, using the preexisting points as centers. The **Circle...** button was clicked in the custom palette. In the **Circle Definition** window as pictured in Figure 34, **Point.7** and **Plane.2** were selected as parameters. The radius was set to 0.25. Then, the full-circle button in the **Circle Limitations** area was clicked. **OK** was clicked, and the circle in Figure 35 was made. This process was repeated for every other plane.

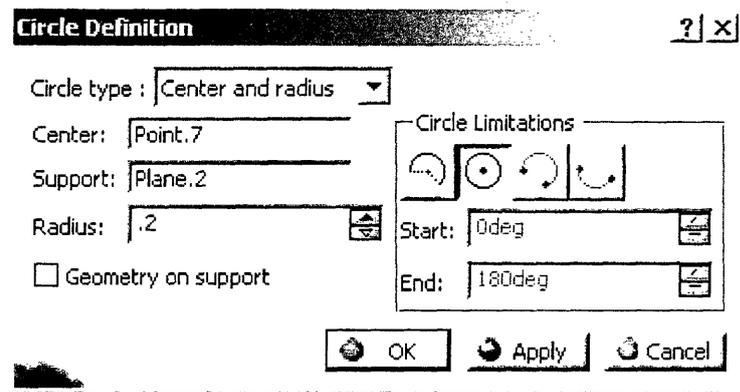


Figure 34: Circle Definition window. The radius was set to 0.20 and the full-circle icon selected.

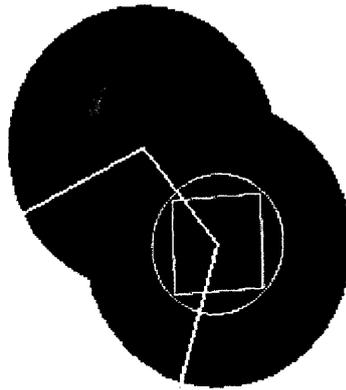


Figure 35: Circle on plane. The circle will be the base of a cylinder that touches two atoms.

Finally, the cylinders were made by extruding the circles along the lines, using the **Extrude...** tool. A length of 1.4 was chosen, as shown in Figure 36, for the cylinder.

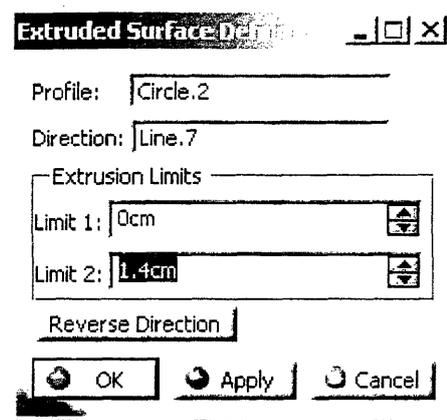


Figure 36: Extruded Surface Definition window. The length of the cylinder, 1.4, is a length that will always connect two spheres in the model.

This was repeated for each circle and line until cylinders were made on all of them. The final figure, the first residue triplet of Collagen 1CGD Chain A, is shown in Figure 37 below.

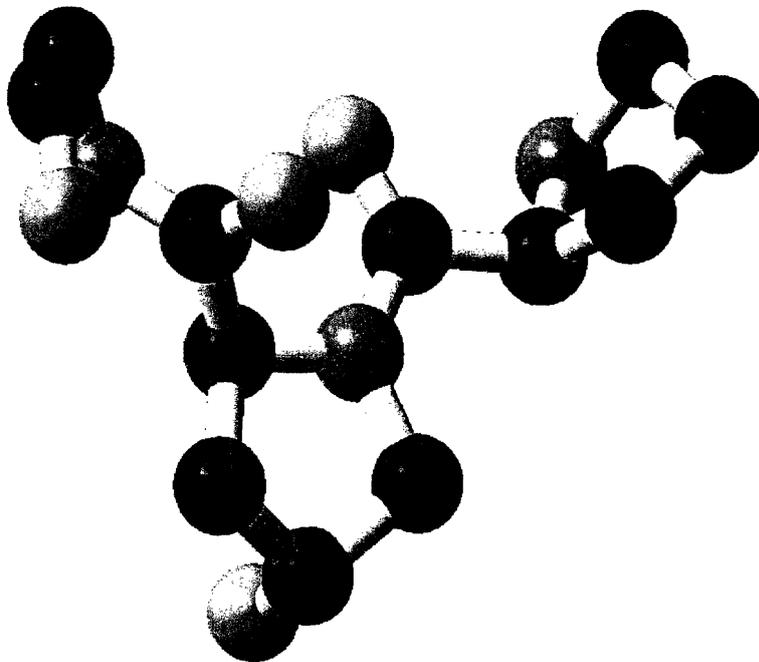


Figure 37: Collagen 1CGD Chain A ball-and-stick model of first residue triplet. This model shows the bonds between the atoms.

The original spheres, **Sphere.1** through **Sphere.19**, were unhidden by right-clicking them in the Tree and selecting **Hide/Show**. Then, they were right-clicked and **Properties** was selected. In the **Graphic** tab, the **Transparency** slider was set to **132**. This made the space-filled spheres semitransparent, showing how the space-filled model fits with the ball-and-stick model. Figure 38 shows the triplet in ball-and-stick mode with a semitransparent space-filled visualization.

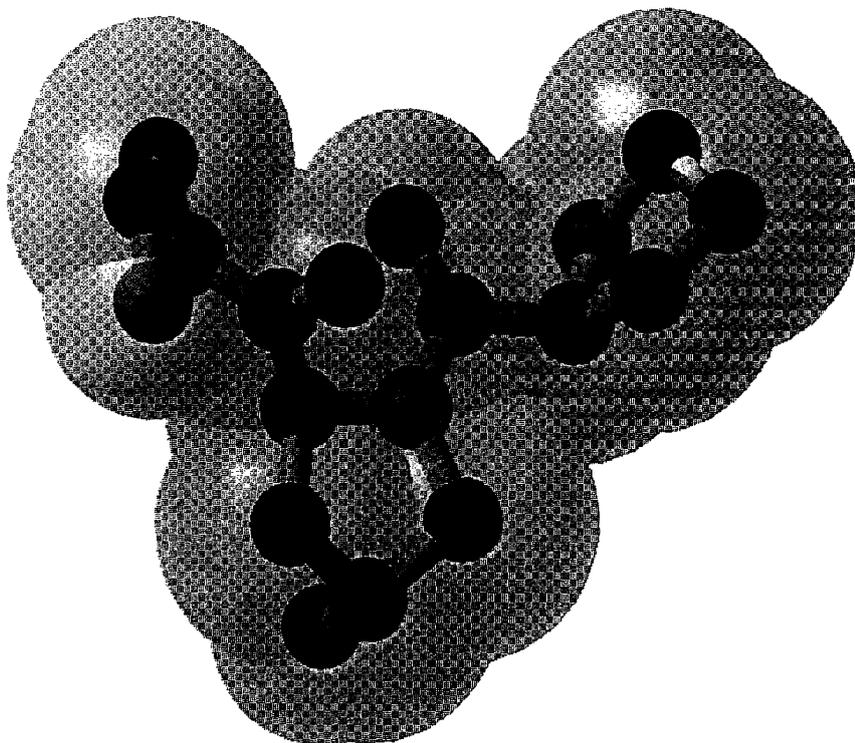


Figure 38: Space-filled and ball-and-stick overlay. This shows the relative sizes of the space-filled spheres and the ball-and-stick spheres. While the ball-and-stick model lacks a true geometric representation, it makes up for this by showing the bonds between atoms much better.

Chapter 6

Conclusions

Space-filled STL files of the three chains for each of Collagen 1BKV and Collagen 1CGD were made. The process to recreate these models or other similar models was painstakingly detailed. A parting line with rigid molds was demonstrated to be infeasible for the geometry of this project. And, a ball-and-stick model for Collagen 1CGD was begun. The process to complete the model was detailed.

I definitely learned much about both SolidWorks and Catia that I had not been exposed to before undertaking this thesis. While I have successfully used SolidWorks in the past to design computer models, I found its resources lacking for this particular project. I found Catia to be a much better tool, but in the process I had to teach myself how to use it. My only experience with Catia software is using a Unix-based version for several months. The difference between that version, Catia V4.2, and the version available on Windows, Catia V5, is quite staggering. The user interface, while still powerful and flexible, changed considerably from its previous counterpart. That said, I would even recommend Catia V4.2, if I had access to it, to continue work on this project. It is able to perform functions, such as making cylinders between any two points in 3D-space, in a single step. As detailed towards the end of Chapter 5, I had to create lines, plains, circles, and extrusions to achieve this same effect. All in all, I would say the solid modeling program experience was quite an adventure and discovery process.

The parting line determination was successfully completed with the help of computer models. An even more detailed analysis could be conducted using a rapid prototyped part and experimenting with mold geometries. After all, if the collagen protein is divided enough times into separate pieces, at some point each of these pieces will be able to be cast in rigid molds. Then, the pieces could be attached to each other after the casting took place. It becomes a question of how many different pieces is acceptable, and if the use of a rigid mold is worth the time and effort it takes to assemble the part.

Additional future work on this project could be directed to completing the ball-and-stick model. However, with this recommendation come some caveats.

Whereas the absolute units of measurement for the space-filled model was irrelevant as long as the relative proportions were held true, this is not the case for the ball-and-stick model. Figure 38 on page 40 shows that the geometry of the spheres and cylinders for the ball-and-stick model is much smaller than that for the space-filled model. One must consider the physical limitations of current manufacturing processes; specifically, can the process accommodate geometry this small? While my thesis did not direct attention at the manufacture process selection, this is nonetheless a very important consideration.

Overall, the efforts of this and Ms. Cofer's thesis produced a working physical model of Collagen 1CGD. Additionally, there are electronic materials for future improvements to the collagen model, or instructions one could follow to design entirely different proteins. Therefore, I would judge that this project successfully fulfilled its goals.

Chapter 7

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