THREE-DIMENSIONAL FINITE-ELEMENT MESH GENERATION FOR THE STUDY OF HEAT CONDUCTION IN LONGITUDINALLY-ALIGNED SHORT-FIBER COMPOSITES

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ABSTRACT

Composite materials are being increasingly used in industrial thermal applications in the last decade; the determination of macroscopic thermal properties of composites is thus of fundamental and practical importance. A frequent and important composite microstructure consists of solid short fibers of circular cylindrical shape dispersed in a solid matrix. Due to manufacturing processes characteristics, an important microstructural model for such composites is that of a periodic cell composed of a short circular cylindrical fiber placed at the center of a cube and along one of its horizontal axes. Finite-element approaches to study heat conduction in short-fiber composites, often developed due to their great geometric flexibility, require the generation of appropriate three-dimensional meshes. In this work, we develop and implement a procedure for generating (tetrahedral) finite-element meshes in the periodic cell; such meshes are then evaluated as to their quality.

Keywords: Mesh Generation, Finite Elements, Short-Fiber Composites, Heat Conduction.

1. INTRODUCTION

Composite materials, or simply composites, are characterized by the presence of several phases and/or dissimilar constituents; often, one component is dispersed as fibers or particles in a continuous matrix of another component. Composites can attain a wide range of thermal properties, and are being continually developed for applications in the aerospace, automobile, and electronic packaging industries; the determination of macroscopic thermal properties of composites, in terms of the microstructure and component properties, is thus of fundamental and practical importance (Mirmira & Fletcher, 1999; Ayers & Fletcher, 1998; Furmanski, 1997). As pointed out by Mirmira & Fletcher (1999), flexible approaches to the study of heat conduction in composites, able to accomodate geometric and physical variations relatively easily, are needed in order to obtain more satisfactory comparison between numerical and experimental studies. Recent advances in computing capabilities have enabled increased accuracy and complexity in numerical simulations; in particular, finite-element approaches (Matt, 1999; Cruz, 1998), which offer great geometric flexibility, require the generation of appropriate two- or three-dimensional meshes.

A frequent and important composite microstructure consists of monodisperse solid thermally-conducting short (chopped) fibers of circular cylindrical shape dispersed in a solid matrix (Mirmira & Fletcher, 1999; Furmanski, 1997). The manufacturing processes for such composites include the step of pressing the components together, such that the fibers tend to align perpendicularly to the applied pressure. As a consequence, the fibers may become either transversely aligned (lying on parallel planes but not parallel to each other in each plane) or longitudinally aligned (lying on parallel planes and parallel to each other). As a first and necessary step to treating the former, more complex, situation, here we consider only the latter situation: to represent the composite, we adopt the microstructural model consisting of a periodic cell composed of a short circular cylindrical fiber placed at the center of a cube and along one of its horizontal axes. The fiber-to-cube volume ratio defines the (dispersed-phase) volume fraction, or concentration, of the composite. The objective of this work is to develop and implement a semi-automatic procedure to generate unstructured three-dimensional (tetrahedral) finite-element meshes in such periodic-cell microstructure. In particular, we develop algorithms for the distribution of finite-element corner-nodes, or simply nodes, on lines and surfaces of the periodic cell; the distributed nodes are subsequently input to a third-party software, which then generates the required surface and volume meshes. The generated meshes are then analysed as to their quality. Future work shall use these volume meshes to calculate the effective conductivity of short-fiber composites; such results are currently lacking, and needed, in the literature (Mirmira & Fletcher, 1999; Furmanski, 1997).

2. UNSTRUCTURED 3-D MESH GENERATION IN THE PERIODIC CELL

Finite-element mesh generation consists in the subdivision of the physical domain of interest in a collection of non-overlapping conforming subdomains, called the elements. Here, our domain is the periodic cell composed of a circular cylindrical short fiber (henceforth denoted simply as fiber) placed at the geometric center of a cubic matrix (the cube) and along its horizontal *X*-axis, as illustrated in Figure 1(a). In the following subsections, we describe our semi-automatic procedure developed to generate unstructured three-dimensional tetrahedral finite elements in the entire volume of the periodic cell. Our procedure consists in six steps: first, nodes are distributed on lines and surfaces of the periodic cell; second and third, surface meshes on the six faces of the cube and on the entire cylindrical surface of the fiber are generated; fourth and fifth, the volume meshes in the fiber and in the region between the cube and the fiber are constructed; finally, the union of these two volume meshes is effected. In order to generate the surface and volume meshes of this work, we use a third-party advancing-front generator, NETGEN 3.2 (Schöberl, 1998; Schöberl, 1997), licensed to the authors for academic use. The six steps are described below.

2.1 Nodes Distribution and Generation of the Surface Mesh on the Cube

We first need to construct a *periodic* surface mesh on all six faces of the cube of side λ containing a fiber of diameter d and length L. The concentration, c, and the aspect ratio, ρ, are nondimensional parameters related to the size of the fiber, and defined as

$$c = \frac{\pi d^2 L}{4\lambda^3}, \quad \rho = \frac{d}{L}. \tag{1}$$

Four fundamental tasks have to be executed in order to generate the desired surface mesh: *periodic* distribution of nodes on the four straight edges of each of two base-faces of the cube; distribution of nodes on the internal contours of the two base-faces; generation of the triangular finite-element mesh inside the base-faces; and, last, appropriate translation and rotation of the two base-faces in order to construct the other four faces of the cube.

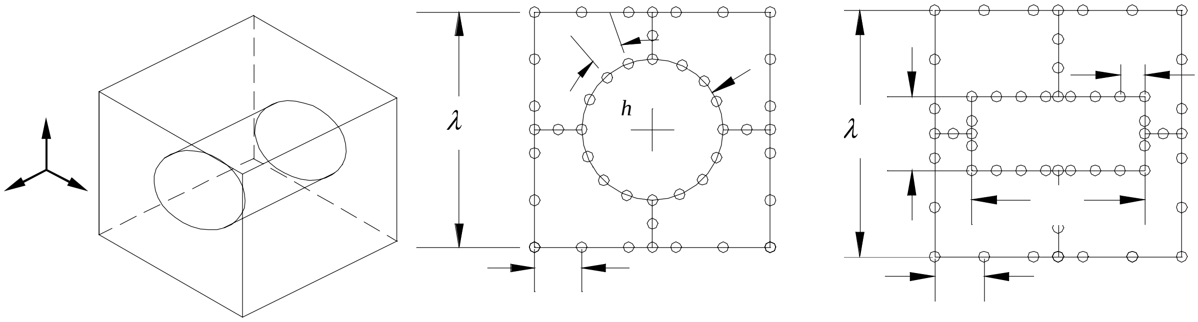
Base-face A, illustrated in Figure 1(b), is a square of side λ containing a circle of radius $d/2$ whose center coincides with the geometric center of the base-face. Base-face B, illustrated in Figure 1(c), is a square of side λ containing a rectangle of sides d and L whose geometric center coincides with the geometric center of the base-face. The regions defined by the circle and the rectangle are the projections of the fiber surface on the respective base-faces. The base-faces *A* and *B* are templates for the faces of the cube normal and parallel to the axis of the fiber, respectively.

The boundary-node distribution function for the lines and internal contours of the base-faces takes into account the physical distance between a boundary node $\boldsymbol{P}_j$ and the solid (fiber) surface in the cell, and is given by

$$h(\boldsymbol{P}_j) = \frac{1}{n_r}\left(\frac{1}{m/d_{\boldsymbol{min}}(\boldsymbol{P}_j) + 1/h_{\boldsymbol{0}}}\right), \tag{2}$$

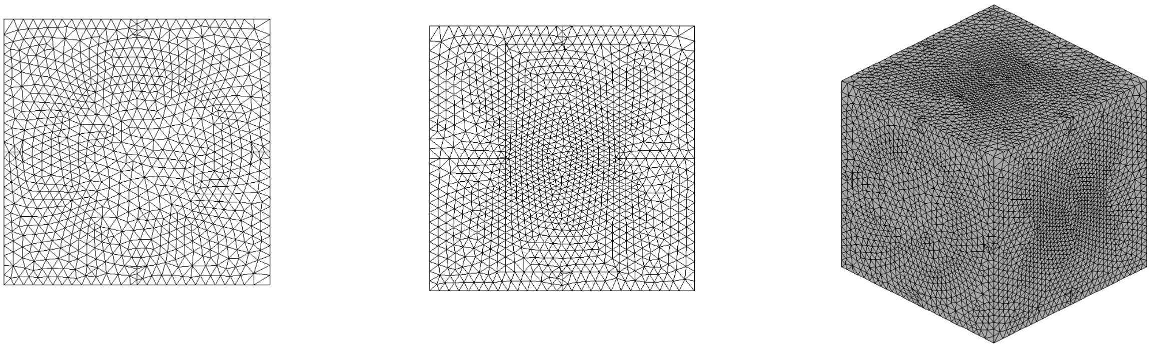
where h is the actual mesh spacing between $\boldsymbol{P}_j$ and the next boundary node $\boldsymbol{P}_{j+1}$, n_r is the global mesh refinement parameter, d_{min} is the minimum distance of the node $\boldsymbol{P}_j$ to the solid surface in the cell, h_0 is the input default mesh spacing, and m is a parameter which guarantees that at least m elements will exist between the node $\boldsymbol{P}_j$ and the solid surface; typically, $m = 2$ and $n_r = 1$ or $n_r = 2$. It is observed that, at high concentrations or high aspect ratios (when $(\lambda - d)/2h_0 < 0.01$ or $(\lambda - L)/2h_0 < 0.01$), the distribution of nodes according to equation (2) leads to the appearance of excessively distorted triangles in the base-faces, mainly in the narrow regions between the edges of the square and the internal contours. We have thus slightly altered the distribution of nodes for these regions: at high values of c or ρ, we insert only one node exactly in the middle of each of the segments that connect the edges of the square to the internal contours (Figures 1(b) and 1(c)). With this modification, a definitive improvement in the quality of the generated triangles is observed. Periodicity of the nodes on the outer edges of the base-faces is guaranteed by the symmetry of our cell geometry.

After the step of distributing nodes on the lines and internal contours of the base-faces, we then pass to the mesh generator NETGEN 3.2, by means of data files, the coordinates and the connectivity of the distributed nodes. The generator then reads these files, and constructs triangular (plane-surface) meshes inside the base-faces, such as the ones illustrated in Figures 2(a) and 2(b). The periodicity around the outer edges of the base-faces can be observed. To enforce cell periodicity, we need to translate and rotate the two base-faces appropriately, so as to construct the other four faces; therefore, opposite faces of the cube are identical. In the *XYZ* Cartesian coordinate system adopted (Figure 1(a)), base-face *A* is a template for the *YZ* faces of the cube, whereas base-face *B* is a template for the *XY* and *XZ* (through rotation) faces. In Figure 2(c), a periodic surface mesh on the cube is shown, obtained with the procedure described above and utilizing the two base-faces illustrated in Figures 2(a) and 2(b).



(a) (b) (c)

Figure 1. (a) Geometry of the cubic cell domain and associated *XYZ* Cartesian coordinate system (a); geometries of the cube base-faces *A* (b) and *B* (c) (not to scale), and respective distributions of nodes on their lines and internal contours, according to equation (2).



(a) (b) (c)

Figure 2. Periodic triangular meshes within the cube base-faces *A* (a) and *B* (b), and periodic cube surface mesh (c) obtained after translations and rotations of the base-faces *A* and *B*; $h_0/\lambda = 0.05$, $m = 2$, $n_r = 1$, $c = 0.25$, $\rho = 2.0$.

2.2 Nodes Distribution and Generation of the Surface Mesh on the Fiber

We now describe the procedure developed to construct the surface mesh on the fiber. The procedure encompasses three fundamental tasks: selection of primitive solids to generate the geometry of the 3-D surface to be meshed, distribution of nodes on selected regions of this surface to be refined, and generation of the triangular finite-element mesh on the surface. The last task is effected by NETGEN 3.2, which is able to triangulate 3-D surfaces allowing for local mesh refinement; the user needs to create a file containing the geometric data relative to the regions to be locally refined.

NETGEN 3.2 has five primitive solids available to the user: plane, sphere, infinite length cylinder, cone, and tube. Here, to generate the geometry of the fiber surface, we need to utilize the infinite length cylinder and the plane. The infinite cylinder is specified through the coordinates of two points on its axis and the radius, $d/2$. The fiber is then specified by means of the intersection operation of the infinite cylinder with two parallel planes normal to its axis, separated by a distance equal to L.

We have implemented an algorithm for the specification of the regions of refinement on the surface of the fiber (lateral surface and bases) and the mesh spacing around the points which define these regions. The regions of refinement are the portions of the fiber surface closer to the other neighboring fibers; these regions are delimited by lines of nodes placed on the lateral surface and on the bases of the fiber, as illustrated, respectively, in Figures 3(a) and 3(b). The nodes distribution function to define the mesh spacing h along the boundaries of such regions is also given by equation (2), but now with d_{min} representing the smallest distance between a node on the fiber surface and the six faces of the cube (note that, due to the longitudinal alignment of the fibers in this work, this distance is proportional to the smallest distance of the node to the surfaces of neighboring fibers). A single data file is then written containing the information on the primitive solids, the (X,Y,Z) coordinates of the nodes distributed on the lines of the regions of refinement, and the mesh spacing h around these nodes.

To accomplish the last task, NETGEN 3.2 reads the data file and subsequently generates a non-uniform triangular finite-element mesh on the surface of the fiber, as illustrated in Figure 4(a). During execution, NETGEN 3.2 prompts the user for the value of the default spacing of the surface mesh; the parameter h_0 is thus entered.

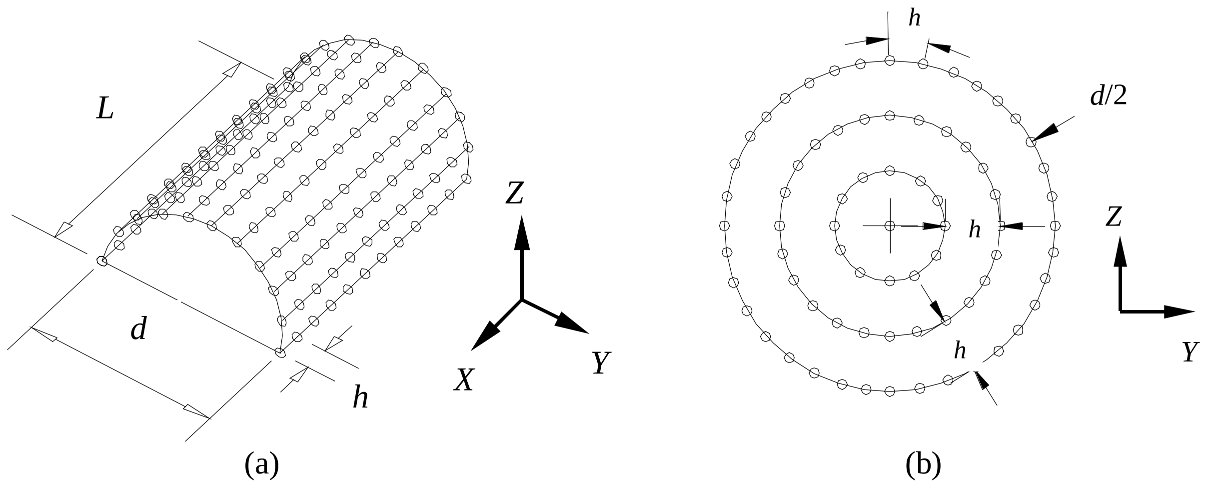


Figure 3. Distribution of nodes along the lines of the regions of refinement on the lateral surface (a) and bases (b) of the fiber.

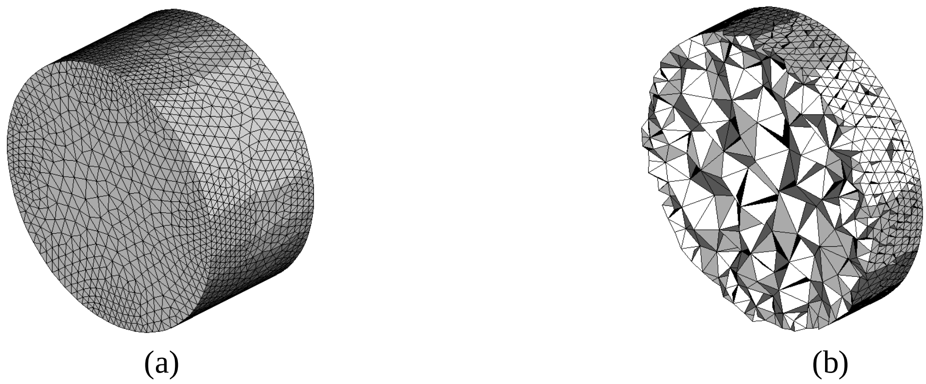


Figure 4. Surface mesh *on* the fiber (a) and *YZ* cross section of corresponding volume mesh *in* the fiber (b); $h_0/\lambda = 0.05$, $m = 2$, $n_r = 1$, $c = 0.25$, $\rho = 2.0$.

2.3 Generation of the Volume Mesh in the Fiber

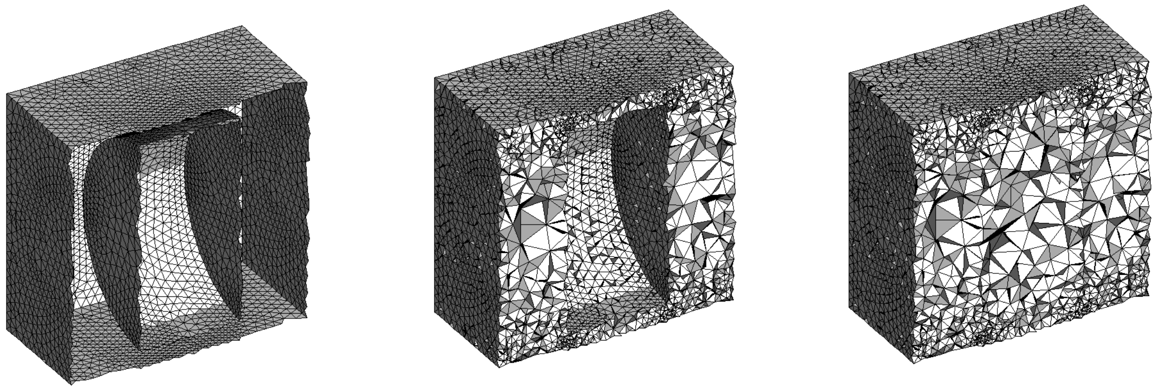
After the generation of the surface mesh on the fiber, as described in the previous section, the geometric information (nodes coordinates) and the topological information (connectivity of triangles) relative to this surface mesh are stored in a data file. Subsequently, this file is read by NETGEN 3.2, which then constructs a tetrahedral volume mesh inside the fiber. Figure 4(b) illustrates a *YZ* cross section of the volume mesh inside the fiber, obtained from the surface mesh shown in Figure 4(a).

2.4 Generation of the Volume Mesh in the Region between the Fiber and the Cube

Following the generation of the periodic surface mesh on the cube and the surface mesh on the fiber, we group all the information relative to these two meshes in a single data file. It is important to remark that, in this step, we have to invert, by node renumbering, the orientation of the triangles of the surface mesh on the fiber, relative to the orientation used generate the volume mesh in the fiber. The data file is then processed by NETGEN 3.2 in order to construct the tetrahedral volume mesh in the region between the fiber and the cube, i.e., in the matrix. Figure 5(a) illustrates the surface meshes on the cube and on the fiber surface, used by NETGEN 3.2 to generate the volume mesh in the region between the fiber and the cube shown in Figure 5(b).

2.5 Union of the Two Volume Meshes

The objective of this last step is to condense the geometric and topological information relative to the two previously generated volume meshes into one single consistent volume mesh inside the whole periodic cell. To accomplish this, we first need to make the two volume meshes compatible at their shared boundary: we thus identify and renumber all the nodes on the fiber surface appropriately, in order to guarantee the same connectivity of nodes of the triangles shared by tetrahedra in the region between the fiber and the cube, and in the fiber. The renumbering is based on the topological, rather than on the geometric, information of the two volume meshes. Finally, the nodes of the volume mesh inside the fiber are renumbered accordingly. A conforming volume mesh inside the periodic cell, obtained from the meshes in Figures 4(b) and 5(b), is shown in Figure 5(c). We note the desired selective refinement of the mesh in the regions where the fiber is closer to the neighboring fibers.



(a) (b) (c)

Figure 5. Surface mesh on the cube and on the fiber (a), volume mesh in the region between the fiber and the cube (b), and *XZ* cross section of corresponding volume mesh in the periodic cell (c); $h_0/\lambda = 0.05$, $m = 2$, $n_r = 1$, $c = 0.25$, $\rho = 2.0$.

3. RESULTS AND CONCLUSIONS

In this section we present and analyse some representative mesh results, and draw some concluding remarks. In Figure 6, we show the surface meshes on fibers of four different periodic cells with varying c, $c \in \{0.10,\ 0.15,\ 0.35\}$, and ρ, $\rho \in \{0.5,\ 2.0\}$. We can clearly see that, as the concentration c increases for fixed aspect ratio ρ, the meshes display the desired selective refinement in the regions where the fiber is closer to the neighboring fibers. The CPU time, in seconds, required to execute the major steps of the procedure for volume mesh generation inside the periodic cells containing the fibers illustrated in Figure 6, is shown in Table 1; the processor is a Pentium II 400 chip with 256 Mb RAM available. We observe that, first, the volume meshes are considerably more time consuming than the surface meshes. Also, as the concentration increases for fixed ρ, the CPU time increases considerably.

The results of standard tests (de l'Isle & George, 1995) conducted to evaluate the quality of the tetrahedra generated by NETGEN 3.2 for the four cell volume meshes of Table 1, are shown in Table 2. An extremely distorted tetrahedron is rated *sliver*, and a regular or equilateral tetrahedron is rated *excellent*. In Table 2, for the four generated cell volume meshes, the number of elements, the number of global nodes, and the percentages of elements rated *sliver*, *bad*, *good* and *excellent* are shown.

Table 1. CPU time, in seconds, required to execute the major steps of the procedure for volume mesh generation inside the periodic cells containing the fibers illustrated in Figure 6; the processor is a Pentium II 400 chip with 256 Mb RAM available.

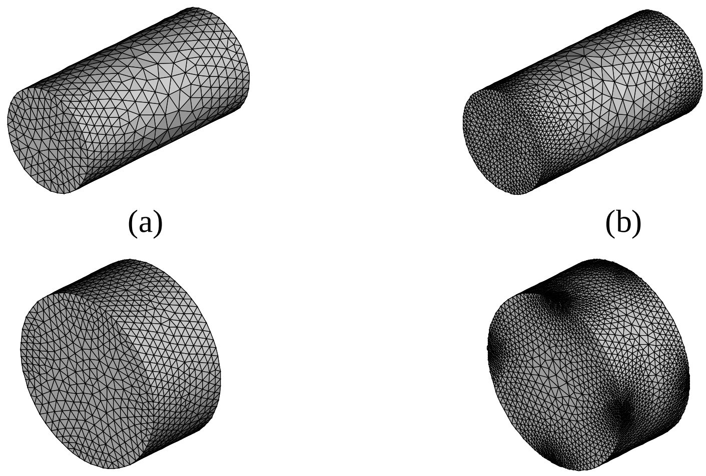
	CPU time, in seconds				
	Base-face *A*	Base-face *B*	Fiber surface	Fiber volume	Matrix volume
6(a)	11	11	12	36	480
6(b)	28	16	48	145	1309
6(c)	9	15	40	66	648
6(d)	9	23	172	505	1452

Table 2. Number of elements, number of global nodes, and percentages of elements rated *sliver*, *bad*, *good* and *excellent* for the four volume meshes generated by NETGEN 3.2 inside the periodic cells containing the fibers illustrated in Figure 6.

	Evaluation tests of the quality of the tetrahedra generated by NETGEN 3.2					
	Number of elements	Number of global nodes	*Sliver*	*Bad*	*Good*	*Excellent*
6(a)	111754	22467	0.2 %	12.0 %	46.0 %	41.8 %
6(b)	177611	33211	1.4 %	11.0 %	43.0 %	44.6 %
6(c)	96328	18508	0.5 %	9.6 %	50.2 %	39.7 %
6(d)	172452	32906	2.1 %	13.0 %	64.1 %	20.8 %

We observe in Table 2 that the presence of excessively distorted tetrahedra is small; nevertheless, they should be eliminated from the mesh. Tetrahedra rated *bad* can be kept in the mesh (Matt, 1999). It is possible that the presence of tetrahedra rated *sliver*, is related to the algorithmic conception of NETGEN 3.2: it is well known in the literature (Baker, 1989) that the *advancing front* algorithms for mesh generation, in spite of representing very well the boundaries of the domain, not always generate elements of acceptable quality inside the domains. Also, it is a fact in unstructured mesh generation that Delaunay triangulation, employed in NETGEN 3.2, offers the best possible triangulation for a given set of nodes in two dimensions; however, this does not apply in three dimensions. Two possible solutions to this problem can be proposed. First, another 3-D mesh generator can be tested in our procedure, preferrably one that utilizes a Voronoi algorithm (Baker, 1989). The second solution, slightly more complex than the first, is to devise and implement an algorithm to identify and fix the distorted tetrahedra, by changing node coordinates; as a consequence, the mesh generated by NETGEN 3.2 would be geometrically, but not topologically, modified.

The procedure developed in this work, to generate meshes for longitudinally-aligned short-fiber composites, can be used in finite-element approaches to solve the heat conduction problem in such materials, in order to determine their effective thermal conductivity. The procedure is also a basis for, and can be extended to, a more sophisticated and realistic microstructural model, that of transversely-aligned short fibers (Mirmira & Fletcher, 1999).



(a) (b) (c) (d)

Figure 6. Fibers, and corresponding surface meshes (h_0/λ = 0.05, m = 2, n_r = 1), of four different periodic cells (not to scale): (a) c = 0.10, ρ = 0.5; (b) c = 0.15, ρ = 0.5; (c) c = 0.15, ρ = 2.0; (d) c = 0.35, ρ = 2.0.

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