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Prediction of structures and mechanical properties of composites using a genetic algorithm and finite element method

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A combined method of a genetic algorithm and finite element stress analysis has been developed to design the structure of materials. The genetic algorithm is applied to searching structures that have a desired property by combining it with the finite element analysis, which is used to predict the elastic modulus and Poisson's ratio. The calculation of the stress analysis is validated from the comparison with the theory on parallel, series, and random structures. The combined method was applied to two searches of structures. One was to find structures that have a desired elastic modulus, respectively. The calculation successfully found a proper structure for each desired elastic modulus. The other was the search of the structure that shows a negative Poisson's ratio. A structure having the negative Poisson's ratio was generated by the calculation. Although this original structure would appear to have no features, it gave us a good idea for the design of materials by investigating the stress distribution in the original structure. A new structure that consists of a unique and continuous pattern of the higher elastic component was designed from the calculation. The reason for the negative Poisson's ratio is explained by mechanical linkage.

1. Introduction

Properties of composites such as polymer alloys, blends, particle-dispersed materials and mixtures, strongly depend on their microscopic structures. Relationship between microscopic structures and macroscopic properties has been experimentally and theoretically investigated by many researchers [1–3]. The basic relation is called the mixture rule, which is a linear mixture equation on a volume basis and is theoretically derived from a parallel structure. Various models for elastic modulus have been summarized by Manson [4] and Ahmed [5]. Now, computer simulation using a finite element method has been used to study on the relation of structures to properties [6–9].

On the contrary, the reconstruction of structures derived from macroscopic properties is also of scientific and practical concern. This is one of the inverse problems. Teraki *et al*. [10] estimated the microstructure of multiphase composites from experimental data on macroscopic properties like elastic modulus by inverse analysis. They assumed that the microstructure were composed of ellipsoidal reinforcements in a continuous matrix and obtained geometric parameters such as the aspect ratio and orientation angle of reinforcements. Recently, genetic algorithms are interested as an evolutionary strategy to improve the adaptability of a system. Gutowski [11] presented a solving for the grain-size distribution for particulate magnetic materials using the genetic algorithm. Byon *et al*. [12] applied the genetic algorithm to optimizing the lamination of hybrid thick-walled cylindrical shell under external pressure. Hartke [13] used the genetic algorithm to optimize the global minimum energy structure of atomic clusters on an empirical potential energy surface. Sugimoto and Li [14] reported an application of the genetic algorithm to the design of the structure composed of composite materials for the reduction of the production cost of the structure. They show that the genetic algorithm is useful for the optimization problem in the material science and engineering.

In this paper, a more attractive application of the genetic algorithm to the materials science and engineering is presented. A combined method of a genetic algorithm and finite element stress analysis has been developed to search structures of composites and mixtures that satisfy desired properties. To investigate the usefulness of the combined method, it was applied to the prediction of elastic moduli of some characteristic structures, finding a structure that have a desired elastic modulus, and the search of a new structure that shows a negative Poisson's ratio.

2. Calculation

2.1. Finite element stress analysis

A finite element stress analysis was applied to predicting the elastic modulus and Poisson's ratio of mixtures

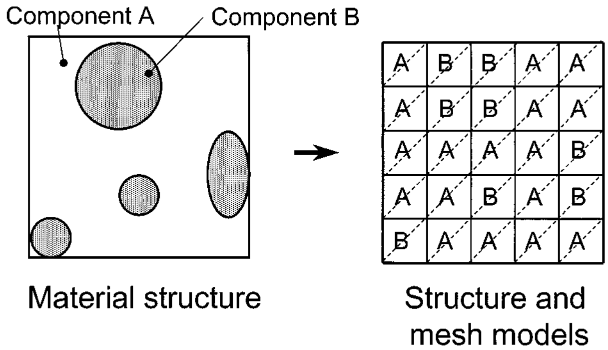

Figure 1 Structure and mesh models for the finite element stress analysis.

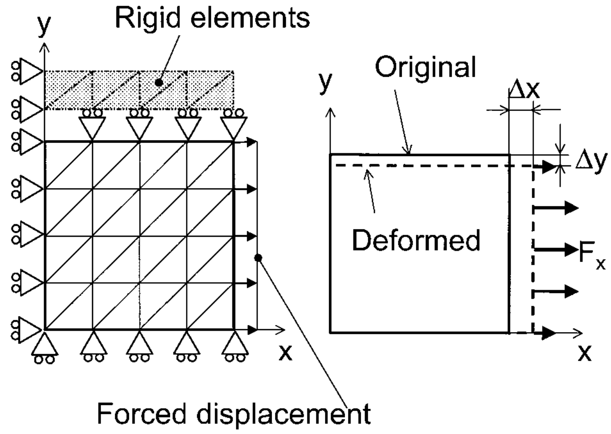

Figure 2 Boundary conditions for the finite element stress analysis.

with complex structures. The structure in a square analysis area with a side length of L is modeled with square grid cells as a structure model as shown in Fig. 1. Each cell is attributed to either component A or component B and then divided into two triangle elements for a mesh model of the finite element stress analysis. The elastic modulus and Poisson's ratio of elements are defined according to the cell attribution. For example, the property data of elements labeled with A are set to be the properties of component A. Fig. 2 shows a mesh model and boundary conditions for predicting elastic modulus and Poisson's ratio in the x-direction. The analysis area is stretched by applying an x-directional forced displacement to the right-hand side. The nodes on the x- and y-axes can only slide in the x- and y-directions, respectively. The rigid elements are virtually introduced out of the area and along the x-direction to keep the top side parallel to the bottom one. Under these conditions and plane stress field, the analysis area will be deformed from square to rectangular like the broken line shape. The displacements of the right-hand and top sides, Δx and Δy, and nodal forces on the right side, F_x, are obtained from the analysis results. By using these values, the x-directional elastic modulus, E_x, and Poisson's ratio, ν_x, are calculated as follows, respectively:

$$E_x = \frac{\Sigma F_x}{\Delta x} \tag{1}$$

$$\nu_x = \frac{-\Delta y}{\Delta x} \tag{2}$$

In a similar way, the y-directional properties are predicted by applying y-directional forced displacements to the top side as follows:

$$E_y = \frac{\Sigma F_y}{\Delta y} \tag{3}$$

$$\nu_y = \frac{-\Delta x}{\Delta y} \tag{4}$$

2.2. Genetic algorithm

The genetic algorithm is combined with the finite element analysis to search the material structure that has a desired property. Fist of all, to apply the genetic algorithm to the material structure design, the structure must be related to a string of genes. The planar structure model is converted to a one-dimensional array as a string of genes as shown in Fig. 3. In the string of genes, components A and B are represented with 0 and 1, respectively.

Fig. 4 shows the flow chart for the combined calculation of the finite element analysis and genetic algorithm. The main process of the genetic algorithm consists of

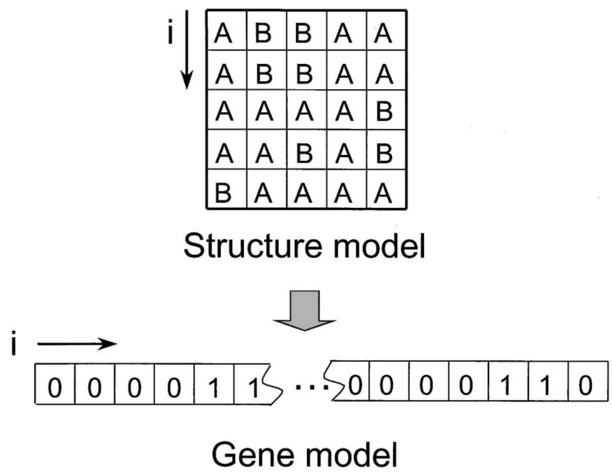

Figure 3 Conversion of a structure model to a string of genes.

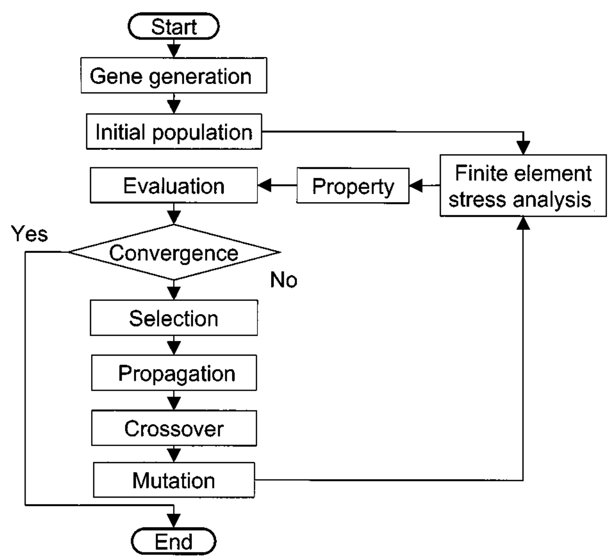

Figure 4 Flow chart for a combined calculation of the genetic algorithm and finite element analysis.

gene creation, initial population, evaluation, selection, propagation, crossover, and mutation. At first, a set of individuals of genes is prepared in the gene generation process. In the initial population, each individual is initialized to be a random structure generated from a different seed as a fist generation of evolution. Then, a target property, the elastic modulus or Poisson's ratio, is calculated for every individual by the finite element stress analysis. The calculated values of the target property of the individuals are compared with the desired one in the evaluation process. The difference between the desired and calculated properties is examined to evaluate the fitness of genes. If the difference is less than the specified criterion, the calculation is finished as almost structures show the target property in this generation. Otherwise, the calculation proceeds the selection. The individuals are sorted in ascending order of the difference and classified into three groups, which are top, middle, and last ones. The individuals that belong to the top group are selected as parents of the next generation. The genes of the parents replace those of the individuals in the last group owing to propagation. Several genes of the copied strings in the last group are randomly changed from 0 to 1 or from 1 to 0 by mutation. For the individuals in the middle group, their genes are partially replaced by those of the parents in the crossover process. Thus, the selection, propagation, crossover, and mutation create a new generation. After that, the stress analysis is carried out for the new generation again. The loop of the stress analysis to mutation is repeated until to obtain the new generation that satisfies the criterion for evaluation.

2.3. Calculation conditions

Calculation conditions for the genetic algorithm and stress analysis are summarized in Table I. The grid size used for the calculation is 20×20 and then the number of cells or genes is 400. The number of individuals is 10. At the initial population, the pseudo-random number generates 10 randomly dispersed structures, which are different each other because unlike seeds are used. The stress analysis is carried out to estimate elastic modulus and Poisson's ratio every structure. The number of parents is 2, which is 20% of the generation. The number of mutants is also 2. The number of genes reversed by mutation is 8, which is 2% of the genes. The number of genes for crossover is automatically decided for each individual by using the random number during calculation.

TABLE I Calculation conditions for the genetic algorithm and stress analysis

Grid size	20×20
Number of individuals	10
Number of genes	400
Number of parents	2
Number of mutants	2
Number of genes for mutation	8
Number of genes for crossover	random
Number of individuals for propagation	2
Initial structures	random
Application 1	
Target property	x-elastic modulus
Target values	2.0, 2.5, 3.0
Elastic moduli (E_B/E_A)	10/1
Poisson's ratios (ν_B/ν_A)	0.4/0.4
Fraction of component B	0.2 (fixed)
Criterion for evaluation	0.001
Application 2	
Target property	x- and y-Poisson's ratio
Target value	−0.3 (both)
Elastic moduli (E_B/E_A)	500/1
Poisson's ratios (ν_B/ν_A)	0.4/0.4
Fraction of component B	0.2 (variable)
Criterion for evaluation	0.01

There are two applications of the genetic algorithm and stress analysis, applications 1 and 2. One is to find a structure that has a desired elastic modulus in the x-direction. Target values are 2.0, 2.5, and 3.0. The elastic moduli of components A and B are 1 and 10, respectively. The fraction of component B is fixed to 0.3 in volume or area. The other is the search of the structure with a Poisson's ratio of −0.3 in both x- and y-directions. The negative Poisson's ratio means that the composites don't shrink but expand transversely if it is stretched. Poisson's ratios of both components are 0.4. It is interesting that composites show negative Poisson's ratios although both components have positive ones. The elastic moduli of components A and B are 1 and 500, respectively. The fraction is 0.2 at the initial stage but is variable in the evolution process. The parameters of evaluation are defined as follows, respectively:

for application 1:

$$\varepsilon_1 = \frac{|E_x - E_d|}{E_d} \tag{5}$$

for application 2:

$$\varepsilon_2 = \frac{(|\nu_x - \nu_d| + |\nu_y - \nu_d|)}{(2\nu_d)} \tag{6}$$

where ε is the error, E is the elastic modulus, and ν is Poisson's ratio. Subscripts 1, 2, x, y, and d indicate applications 1 and 2, directions x and y, and the desired value, respectively. The criteria of evaluation are 0.001 for application 1 and 0.01 for application 2.

The calculation parameters were decided after several trial calculations. A workstation (IBM RS6000-590) and our own FORTRAN program were used for calculations.

3. Results

3.1. Prediction of elastic modulus using the finite element method

The finite element stress analysis is verified by comparing calculated values with theoretical ones on elastic modulus. The parallel model and the series model are well known to estimate properties of composites. They are very simple but often used for discussion because they are basic of the prediction of material properties. The elastic moduli of parallel model and series one are theoretically represented as the following equations, respectively:

parallel model:

$$E_C = E_A f_A + E_B f_B \tag{7}$$

series model:

$$E_C = \frac{E_A E_B}{(E_A f_B + E_B f_A)} \tag{8}$$

where f is the volume fraction and $f_A + f_B = 1$. Subscripts A, B, and C indicate component A, component B, and the composite, respectively. For a random structure, the calculation is compared with Hirsch model.

Hirsch model:

$$E_C = \chi(E_B f_B + E_A f_A) + (1 - \chi)\frac{E_B E_A}{(E_B f_A + E_A f_B)} \tag{9}$$

where χ is the experimental parameter and is here assumed to be the same as the volume fraction of component B. Fig. 5 shows the structure used for the finite element analyses. This structure is generated using the pseudo-random number.

Fig. 6 shows the comparison between calculation and theory in elastic modulus when $E_A/E_B = 1/10$ and $\nu_A = \nu_B = 0.4$. The normalized elastic modulus E_C/E_A is plotted against the volume fraction of component B. The elastic modulus of the parallel model lineally increases with increasing volume fraction because the parallel model corresponds to the simple additive rule. The value of the series model is smaller than that of the parallel one. The curve of Hirsch model for the random structure is located between those of parallel and series models because Hirsch model is a hybrid of parallel and series ones. In every case, the calculated results are in good agreement with the theoretical ones in the whole range of the fraction. As the results of the comparison, it was recognized that the finite element stress analysis gives us reasonable predictions.

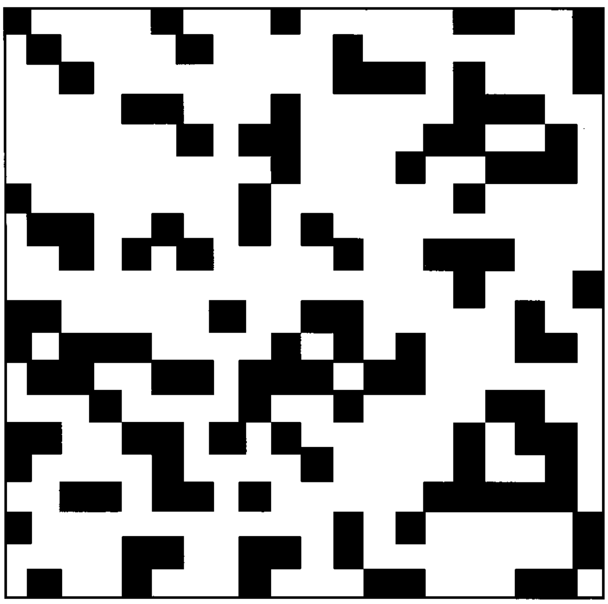

Figure 5 Randomly dispersed structure model (white: component A, black: component B).

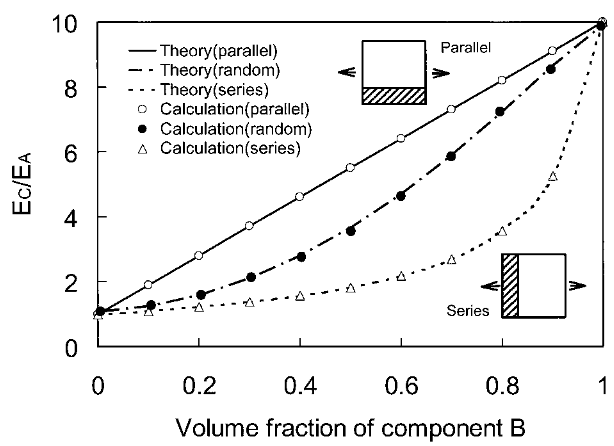

Figure 6 Comparison between calculation and theory in elastic modulus for parallel, series, and random structure models.

3.2. Search of structures with a desired x-elastic modulus

An average error during the genetic algorithm calculation is shown in Fig. 7. The average error is obtained from errors of all individuals except mutants and is plotted against the number of generation. The desired elastic moduli are 2.0, 2.5, and 3.0 in the x-direction under a constant fraction of 0.3. The average error decreases with an increase in generation every property. Since the criterion for evaluation is 0.001, every calculation is successfully finished. The error is twice below the criterion to make sure of the convergence. The generation is the shortest when $E_x = 2.0$ and the longest when $E_x = 3.0$. The number of the generation is due to the difference between the initial structures and findings. The structures found by the calculation are illustrated in Fig. 8. Filled cells refer to component B. Their textures seem to be granular for $E_x = 2.0$, dendritic for $E_x = 2.5$ and lamellar for $E_x = 3.0$. From these textures, the final structure is similar to the initial one for $E_x = 2.0$

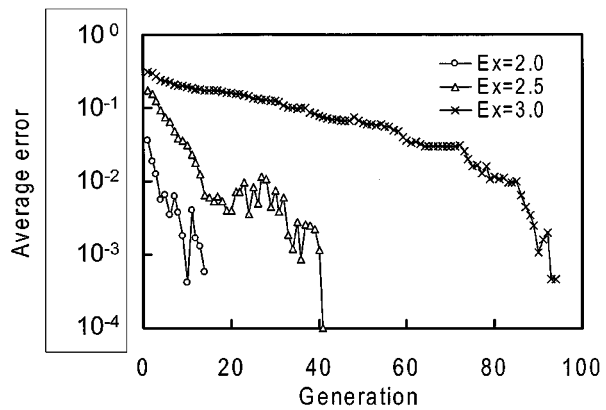

Figure 7 Evolution process during the search of structures with desired x-elastic moduli.

Figure 8 Calculated structures with desired x-elastic moduli (white: component A, black: component B).

but significantly different from that for $E_x = 3.0$. If the parallel model is included in the first generation as an initial individual, the solution can be obtained faster in the case of $E_x = 3.0$.

The elastic moduli are 1.37 for the series model and 3.7 for parallel one. When the desired elastic modulus was smaller than 1.37 or larger than 3.7, the calculation did not find any structures. For the desired elastic moduli between 1.37 and 3.7, the genetic algorithm found the proper structures. These results are consistent with the idea that the series model indicates the minimum value and the parallel one indicates the maximum value.

3.3. Search of structures with a negative Poisson's ratio

The average error for evaluation plotted against the generation is shown in Fig. 9. The average error decreases gradually with increasing generation until 50 generations and, after that, drops systematically because of the action of mutants. The calculation is successfully finished at 142 generations. Fig. 10 shows the structure found by the calculation. Since the fraction is variable, its fraction becomes 0.41. The elastic modulus is 11.1 close to that of component A. As expected, this structure can show a negative Poisson's ratio of -0.3 in both x- and y-directions although the structure seems to have no features. The reason for the negative Poisson's ratio is discussed by investigating the stress distribution. Selecting cells where the absolute value of stress is higher than the average one draws the center illustration in Fig. 11. By eliminating extra cells from the original structure, a singular network appears. It is thought that this network is important to course the negative Poisson's ratio. Since this structure gives us a good idea, we can easily design the right-hand structure by modification. The fraction of this designed structure is 0.13. Although the designed structures would appear to be quite different from the original one, they are essentially similar in the stress field.

To confirm that the designed structure shows the negative Poisson's ratio, a detailed stress analysis for the designed structure was carried out using a fine grid of 60×60. The predicted Poisson's ratios are shown in Fig. 12 against the ratio of elastic modulus, E_B/E_A. The x- and y-Poisson's ratios decrease with increasing ratio of elastic modulus. It is noted that two Poisson's ratios almost agree with each other in spite of asymmetric structure on rotation. Both Poisson's ratios become zero at about 60 in the ratio of elastic modulus. This means that such system shows a constant width when it is stretched. Furthermore increasing the ratio of elastic modulus, both Poisson's ratios are negative. When the ratio of elastic modulus is in vicinity of 150, this system shows the desired Poisson's ratio of -0.3. Fig. 13 shows the predicted elastic modulus for the designed structure. The predicted elastic modulus increases with increasing ratio of elastic modulus but its rise is small. The elastic modulus of the system strongly depends on that of component A or the matrix. The x- and y-elastic moduli are nearly equal.

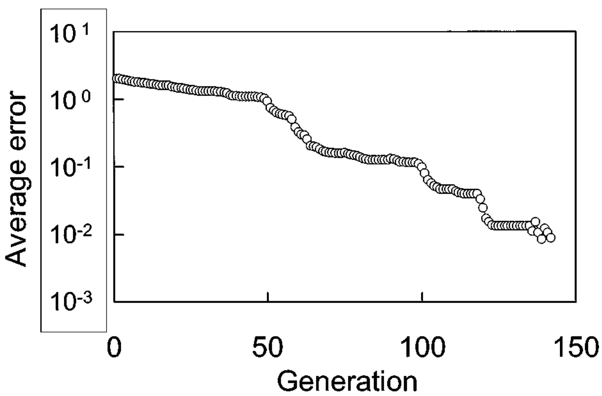

Figure 9 Evolution process during the search of structures with a negative Poisson's ration.

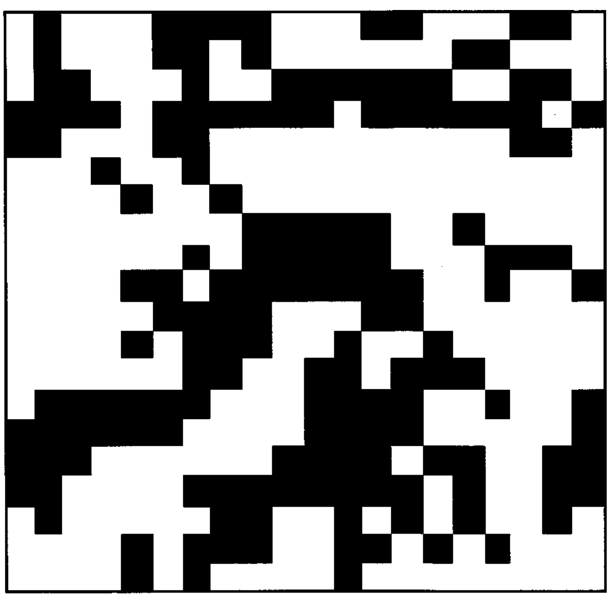

Figure 10 Structure originally found by calculation for showing a negative Poisson's ratio (white: component A, black: component B).

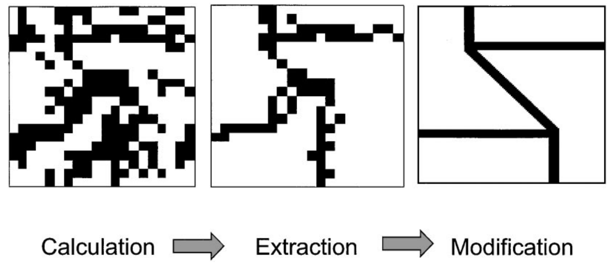

Figure 11 Extracted and designed structures from the original one.

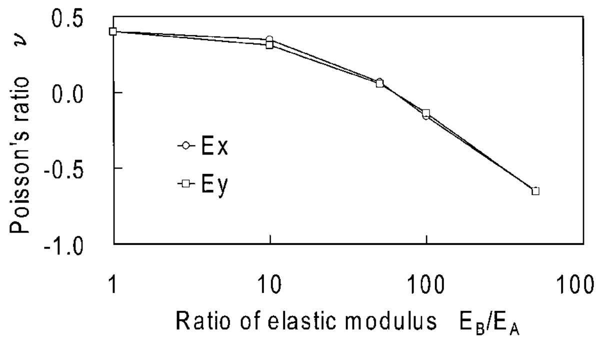

Figure 12 Predicted Poisson's ratio of the designed structure.

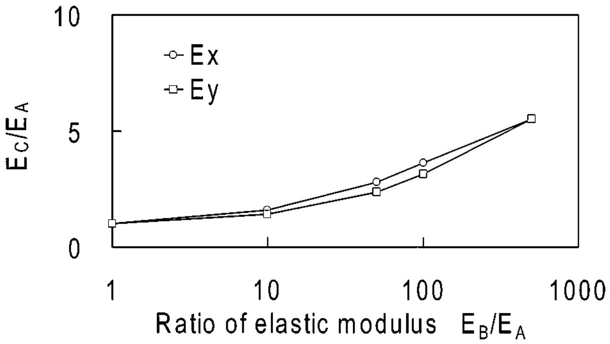

Figure 13 Predicted elastic modulus of the designed structure.

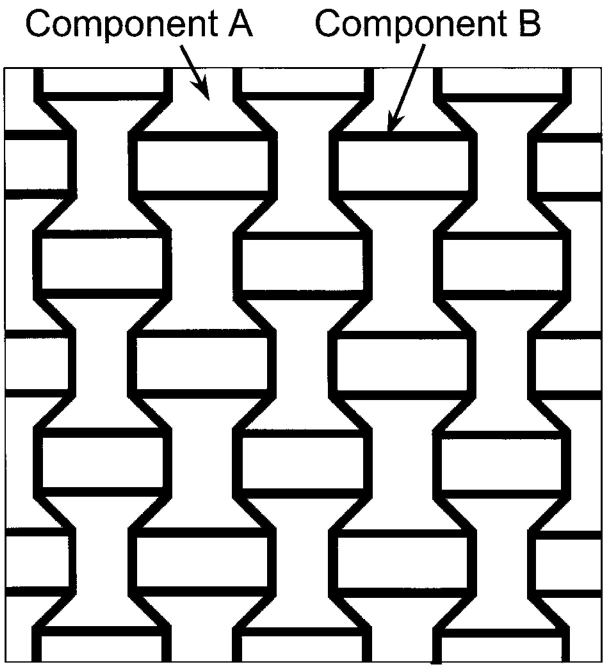

Figure 14 Cyclic pattern of the designed structure that shows a negative Poisson's ration.

3.4. Discussion

As described above, we designed a new structure that causes negative Poisson's ratio from the results calculated by the genetic algorithm and stress analysis. The structure illustrated in Fig. 11 is a quarter of the designed structure because of the boundary conditions for the stress analysis. The full structure is shown in Fig. 14, which is drawn by reflecting the quarter structure 6 times in the x- and y-directions according to the boundary conditions. We can see a unique and continuos pattern in the structure and then understand reason for the negative Poisson's ratio from the pattern. The negative Poisson's ratio is mechanically caused by linkage of component B. When the structure is transversely extended, the curved vertical bars are pulled and longitudinally expanded by the horizontal ones. On the contrary, by stretching the curved vertical bars longitudinally, they push the horizontal bars like expanding the structure transversely. Therefore the elastic modulus of the component that composes the pattern must be much larger than that of the matrix. Elastic moduli of typical materials are summarized in Table II. E/E_{PP} is the ratio of each elastic modulus against that of polypropylene and E/E_{RB} is against rubber. To compose the material having a Poisson's ratio of -0.3, the elastic modulus of the pattern is necessary to be 150 times larger than that of the matrix from the stress analysis. There are two couples in the table. One is the composition of polypropylene as the matrix and steel as the pattern. The other is of rubber and polyethylene. The outline of the composition is a system that consists of metals and plastics including rubbers. To realize the material having a negative Poisson's ratio, the following constructions are suggested: (1) a metal foil with the designed pattern is laminated with a polymer film, (2) the pattern is directly drawn on a polymer film by vacuum vapor depositing and metallizing.

TABLE II Elastic moduli of typical materials

Materials	Elastic modulus E (MPa)	Ratio E/E_{PP}	Ratio E/E_{RB}
Glass	71	55	14260
Aluminum	70	54	14060
Steel	210	162	42000
Copper	130	100	26000
Polypropylene (PP)	1.3	1	260
Polyethylene	0.67	1	134
Nylon66	2.30	2	460
Rubber (RB)	0.005	0	1
Epoxy resin	2.4	2	480
Wood	13	10	2600

4. Conclusion

A combined method of a genetic algorithm and finite element stress analysis has been developed to design the structure of materials. The finite element stress analysis was used to predict the elastic moduli of composites with parallel, series, and random structures. The predicted results were in good agreement with the values estimated by theoretical models. From this comparison, it was recognized that the finite element stress analysis gives us reasonable predictions. The combined method was applied to two searches. One was to find three structures that have a desired elastic modulus, respectively. The calculation successfully found the proper structure for each desired elastic modulus. The other was the search of structures that show a negative Poisson's ratio. The calculation demonstrated a structure with the negative Poisson's ratio. Although this original structure would appear to have no features, it gave us a good idea for the design of the structure by investigating stress distribution. A new structure that consists of a unique and continuous pattern of one of the components has been designed from the calculation. The reason for the negative Poisson's ratio is explained by mechanical linkage. The composition of metals as the pattern and plastics as the matrix has been suggested to realize the material that has a negative Poisson's ratio.

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