Comparison of volume constraint and mass constraint in structural topology optimization with multiphase materials

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Abstract
Instead of adopting the common idea of using volume constraint in topology optimization, this work is focused on the structural topology optimization of multiphase materials with mass constraint. Related optimization models involving mass constraint and interpolation model are proposed. GSIMP (generalized Solid Isotropic Material with Penalization) and UIM (Uniform Interpolation Model) interpolation schemes are discussed and compared. The former is found to introduce the nonlinearity into the mass constraint and brings numerical difficulty to search the global optimum of the optimization problem. The adopted UIM scheme makes it possible to have a linear expression of mass constraint with separable design variables. This favors very much the mathematical programming approaches, especially the convex programming methods. Numerical examples show that the presented scheme is reliable and efficient to deal with the topology design problems of multiple materials with mass constraint. The latter is proved to be more significant and practically meaningful than the volume constraint in structural topology optimization of multiphase materials.
Keywords: topology optimization; multiphase materials; volume constraint; mass constraint

1. Introduction

Structural topology optimization has been extended to various complicated design problems in recent years, such as the design-dependent load and multiple-field problem. In structural topology optimization, the material interpolation model is needed to transform the discrete design problem into a continuous one. Most popular schemes include the SIMP (Solid Isotropic Material with Penalization), RAMP (Rational Approximation of Material Properties) and homogenization method. Until now, most works of the topology optimization and the material interpolation model have been concerned with only one single solid material.

In 1992, Thomsen [1] began to study the structural topology optimization with multiple materials and then many researches were made about these design problems. Sigmund [2, 3] expanded the SIMP model to interpolate the material properties in the optimization problems with two solid materials and void, and the model was adopted in the design of the compliant mechanisms and the microstructure with extreme thermal expansion coefficient. Later, Sun and Zhang [4, 5] applied the same material interpolation model on the multi-objective optimization design of the microstructure, and the perimeter control method was improved to avoid the checkerboard pattern. This model also was used by Gao and Zhang [6, 7] to solve the topology optimization problems with multiple materials under pressure and thermal stress loads.

Yin and Ananthasuresh [8] used the so-called peak function to interpolate the properties of multi-phase materials. The main advantage of that model is its ability to include multiple materials without increasing the number of design variables. However, for more than two materials, the peak function model has some nonlinear difficulties in the numerical procedure. The authors suggested that the standard deviation of the peak function should gradually decrease after each optimization iteration. Wang and Zhou [9, 10] applied the phase field method for topology optimization of multi-material structures. A generalized Cahn–Hilliard model was introduced to transform the structural optimization problem into a phase transition problem. Mei and Wang [11] introduced the level set to achieve the optimal shape and topology with multiple materials. The structural material interfaces were implicitly described by the vector level set and evolved continuously in the structure. Han and Lee [12] presented a material mixing method for ESO (Evolutionary Structural Optimization). The idea is very easy to understand. Considering the elements with low strain energy in ESO, if the element is filled with the larger stiffness material, it should be changed to the lower stiffness material; only the element with lower stiffness material will be removed. In the work of Stegmann and Lund [13], the laminate design with candidate fiber orientations was treated as the discrete material optimization (DMO) problem and tested with several interpolation models.

Until now, although both the structural (e.g. minimization of structural compliance) and micro-structure (e.g. micro-structure design to minimize the thermal expansion coefficient or maximize the elastic modulus) design problems were investigated, the volume constraint has been defined to limit the material amount. For the

optimization problem with one phase solid material and void, the volume and mass constraints are exactly equivalent; nevertheless, they are totally different for the case of multiple solid materials.

In this paper, the topology optimization problem of multiple materials with mass constraint is investigated. Two types of material interpolation schemes are considered, and the corresponding expressions of the optimization problem and the volume constraints are presented. Then the interpolation models of the material density and the expressions of the mass constraint are introduced. Numerical examples are presented to illustrate the validity of the presented interpolation scheme for multiple materials and the optimization model with mass constraint. Numerical tests and theoretical analysis are made to compare both types of interpolation schemes. The mass constraint is proved to be more significant and important than the volume constraint in structural topology optimization.

2. Volume constraint and material interpolation model of multiple materials

In this section, consider the traditional structural topology optimization problem, such as the minimum-compliance design with multiple materials subjected to the volume constraint. Obviously, for this type of problem, only the interpolation model of the Young's modulus is needed. The material interpolation models aim at relating the design variable to the properties of the candidate materials. Usually, in the final optimization result, the mixed property should be equal to that of one certain candidate material. Here, two types of material interpolation schemes are investigated.

2.1 Generalized SIMP model (GSIMP)

This model was introduced by Bendsoe and Sigmund [14]. For the problems with m solid materials, each element will have m number of design variables.

For the case of one solid material, the interpolation model of Young's modulus is expressed as

$$E_i = E(\mathbf{x}_i) = x_{i1}^p E^{(1)}$$
$$\mathbf{x}_i = \{x_{ij}\} \quad (i=1,...,n; \quad j=1) \tag{1}$$

where x_{i1} is the topology design variable of element i, which represents the existence of the solid material or void.

The topology optimization problem to minimize the structural compliance should be written as

$$\begin{aligned}
&\text{find: } \{x_{i1}\} \quad (i=1,...,n)\\
&\text{minimize: } C = \mathbf{F}^T\mathbf{u}\\
&\text{subject to: } \mathbf{F} = \mathbf{K}\mathbf{u}\\
&\quad 0 < x_{min} \le x_{i1} \le 1\\
&\text{volume constraint: } \sum_{i=1}^n V_i x_{i1} \le vf_1 \cdot \sum_{i=1}^n V_i
\end{aligned} \tag{2}$$

where vf_1 is the prescribed volume fraction of the solid material 1. V_i denotes the volume of element i. Usually, a lower bound, x_{min}, e.g., 10^{-3}, is introduced for the design variables to avoid the singularity of the structural stiffness matrix in the finite element analysis.

The SIMP model can be easily extended to the case of two solid materials. For this case, two design variables x_{i1} and x_{i2} are assigned to element i

$$E_i = E(\mathbf{x}_i) = x_{i2}^p \left(x_{i1}^p E^{(2)} + (1 - x_{i1})^p E^{(1)} \right)$$
$$\mathbf{x}_i = \{x_{ij}\} \quad (i=1,...,n; \quad j=1,2) \tag{3}$$

$x_{i2} = 1$ represents the existence of either solid material 1 or 2, while x_{i1} determines which phase the element is. $x_{i2} = 0$ represents the element is void regardless of the value of x_{i1}. Similarly, the structural topology optimization problem can be stated as

$$\begin{aligned}
&\text{find: } \{x_{i1}, x_{i2}\} \quad (i=1,...,n)\\
&\text{minimize: } C = \mathbf{F}^T\mathbf{u}\\
&\text{subject to: } \mathbf{F} = \mathbf{K}\mathbf{u}\\
&\quad 0 < x_{min} \le x_{ij} \le 1 \quad (j=1,2)\\
&\text{volume constraint: } \sum_{i=1}^n V_i x_{i2} \le (vf_1 + vf_2) \cdot \sum_{i=1}^n V_i\\
&\quad \sum_{i=1}^n V_i x_{i1} \le vf_2 \cdot \sum_{i=1}^n V_i
\end{aligned} \tag{4}$$

In this expression, it should be noticed that the constraints of material amount are expressed as two volume

constraints to favor the problem resolution. The first one is to limit the total volume of solid phases 1 and 2, while the second one is to control the solid phase 2. In this manner, the volume constraints will hold a separable and linear form in terms of both sets of design variables.

The same reasoning can be made for the optimization problems with m solid material problem to establish the material interpolation model and the volume constraints.

2.2 Uniform interpolation model (UIM)

This type model was introduced and studied by Stegmann and Lund [13] firstly. In their paper, the laminate design problem with candidate fiber orientations was treated as the discrete material optimization (DMO) problem, and several expressions of this type model were presented and analyzed. For each designable element, each phase solid material corresponds to a topology design variable and all these design variables are uniform. Thus, this type model is named as the uniform interpolation model in this paper. Obviously, each element will have m number of design variables for the case of m solid materials.

The UIM interpolation model of the Young's modulus can be expressed as the weighted sum of all candidate material

$$E_i = \sum_{j=1}^{m} w_{ij} E^{(j)} \tag{5}$$

where w_{ij} is the weight corresponding to the *jth* phase material. To make sure that the unique material exists in each single designable element, a series of constraints as expressed below have to satisfy.

$$\sum_{j=1}^{m} w_{ij} \leq 1 \tag{6}$$

The structural topology optimization problem with volume constraints can be stated as

$$\begin{aligned}
&\text{find:} && \{x_{ij}\} \quad (i=1,...,n; \quad j=1,...,m)\\
&\text{minimize:} && C = \mathbf{F}^{\mathrm{T}}\mathbf{u}\\
&\text{subject to:} && \mathbf{F} = \mathbf{Ku}\\
& && 0 < x_{\min} \leq x_{ij} \leq 1\\
& && \sum_{j=1}^{m} w_{ij} \leq 1\\
&\text{volume constraint:} && \sum_{i=1}^{n} V_i x_{ij} \leq vf_j \cdot \sum_{i=1}^{n} V_i
\end{aligned} \tag{7}$$

Varity of the expression of w_{ij} can be adopted. Numerical tests show that there always are many elements with mixed material in the optimization result for the case of $w_{ij} = x_{ij}$. Thus, several other expressions of w_{ij} will be discussed as below.

(a) UIM-1

$$w_{ij} = x_{ij}^{p} \tag{8}$$

w_{ij} is defined as the penalization of the design variable. Our tests show that this model can not yield a 0-1 solution and there exists middle density area. As concluded by Stegmann and Lund [13], this model "is not very efficient as it fails to push the design to its limit values". To push the design variables towards the bound, an additional term $a\sum_{i=1}^{n}\sum_{j=1}^{m} x_{ij}\left(1-x_{ij}\right)$ is attached to the objective function. Here, a is the prescribed weight. The suitable a can lead to black-white topological configuration. The phase field method presented by Wang and Zhou [9, 10] is actually similar to UIM-1 with the additional term.

Another disadvantage of UIM-1 is that a series of constraints as expressed in eq. (6) have to be included in the optimization problem to make sure the unique material exists in each single designable element. Obviously, the number of these constraints equals the designable element numbers. The large number of both the design variables and the constraints will bring more difficulties for the mathematical programming approaches.

(b) UIM-2

$$w_{ij} = x_{ij}^{p}\prod_{\substack{\xi=1\\ \xi\neq j}}^{m}\left(1-x_{i\xi}^{p}\right) \tag{9}$$

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This model was introduced by Stegmann and Lund (2005). For each design variable, we have $0 \leq x_{ij} \leq 1$. Then, $w_{ij} = 1$ if $x_{ij} = 1$ and $x_{i\xi} = 0$ $(\xi \neq j)$. Similarly, $w_{ij} = 0$ if $x_{ij} = 0$ or $x_{i\xi} = 1$ $(\xi \neq j)$. Thus, we must have $w_{i\xi} = 0$ $(\xi \neq j)$ if $w_{ij} = 1$, which means the element consist of one single phase solid material. Accordingly, UIM-2 overcomes the drawbacks of UIM-1. In other words, UIM-2 can yield 0-1 solution and each designable element consists of one phase material without the additional constraints in eq.(6).

(c) UIM-3

$$w_{ij} = \frac{x_{ij}^p \prod_{\substack{\xi=1 \\ \xi \neq j}}^m \left(1 - x_{i\xi}^p\right)}{\sum_{\varsigma=1}^m x_{i\varsigma}^p \prod_{\substack{\xi=1 \\ \xi \neq \varsigma}}^m \left(1 - x_{i\xi}^p\right)} \tag{10}$$

The optimization cannot converge if this model is used to the Young's modulus. Stegmann and Lund [13] concluded that this model should be only used to interpolate the mass constraint.

3. Mass constraint and material interpolation model of multiple materials

For the structural topology optimization subjected to the mass constraint, the interpolation scheme of the density has to be involved. For a meshed structure with n designable finite elements, the mass constraint can be stated as

$$\sum_{i=1}^n \rho_i V_i \leq \overline{M} \tag{11}$$

where ρ_i is the density of the element i and $\overline{M}$ is the upper bound of the structure mass. Then, the topology design problem to minimize the structural compliance should be written as

find: $\{x_{ij}\}$ $(i = 1, ..., n; \quad j = 1, ..., m)$

minimize: $C = \mathbf{F}^T \mathbf{u}$ $\hspace{3cm}$ (12)

subject to: $\mathbf{F} = \mathbf{K}\mathbf{u}$

$\hspace{2cm} 0 < x_{\min} \leq x_{ij} \leq 1$

$\hspace{2cm}$ mass constraint: $M = \sum_{i=1}^n \rho_i(x_{ij}) V_i \leq \overline{M}$

Firstly, consider the GSIMP model. For the problem of one solid material, the volume constraint and the mass constraint are exactly equivalent. If two solid materials are available, like the interpolation of the Young's modulus in eq.(3), the density of the mixed material can be formulated as

$$\rho_i(x_{ij}) = x_{i2}\left(x_{i1}\rho^{(2)} + \left(1 - x_{i1}\right)\rho^{(1)}\right) \tag{13}$$

Obviously, this expression is variable-inseparable and nonlinear. These characteristics bring numerical difficulties to search the global optimum of the optimization problem when the popular convex approximations are used, such as ConLin [15], MMA [16], GCMMA [17] and MDQA [18]. Some illustrations will be presented in the next section. For the UIM interpolation model with m phase solid materials, ρ_i can be formulated as a linear expression

$$\rho_i = \sum_{j=1}^m x_{ij} \rho^{(j)} \tag{14}$$

In this formulation, the design variables are obviously separable. This favors very much the mathematical programming approaches, especially the convex programming methods.

In all numerical examples of this paper, if GSIMP scheme is adopted, the Young's modulus and density are interpolated using eq.(1, 3) and eq.(13), respectively; while eq.(9) and eq.(14) are applied for UIM-2 scheme. For both schemes, the mass constraint is described in eq.(11).

4. Numerical examples

In this section, Both GSIMP and UIM-2 models are applied to solve the minimum compliance structure design problem. Suppose four "virtual" isotropic solid materials are available in design and they have different stiffness-to-mass ratios.

Table 1 Properties of the virtual materials

virtual material	Young's modulus (GPa)	density (kg/m3)	stiffness-to-mass ratio
VM1	70	2700	0.0259

VM2	210	5400	0.0389
VM3	105	5400	0.0194
VM4	175	3600	0.0486

4.1 Cantilever beam under a load on the right-bottom corner

A cantilever beam example is presented here, as shown in Fig.1. The structure is uniformly meshed with 80×50 elements. Consider two solid material (VM2 and VM1). The mass constraint is set to be $\overline{mass} = 70 \times 10^3 \, kg$ and the optimization results of GSIMP and UIM-2 are shown in Fig.2.
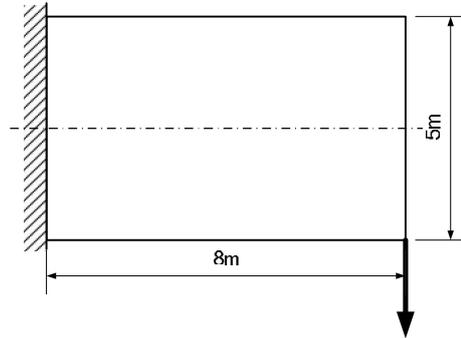

Fig.1 Cantilever beam under a load on the right-bottom corner

As shown in Fig.2(a), the optimal structure using GSIMP model consists of both VM1 and VM2. As a comparison, the result with single solid material (VM2) is shown in Fig.2(b). Obviously, the structure with VM2 is stiffer. Then it can be found that GSIMP model may not yield the global optimization result. The optimal structure using UIM-2 model of VM2-VM1 is shown in Fig.2(c) and only VM2 remains. The configurations in Fig.2(c) and Fig.2(b) are very similar and the structure compliances using UIM-2 is even smaller.

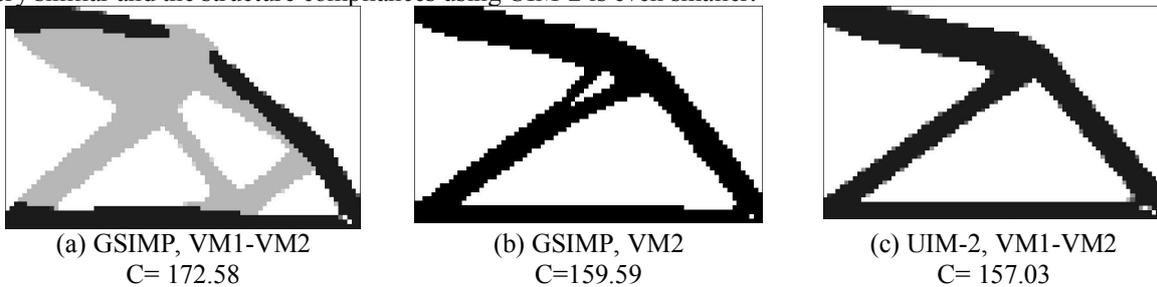| (a) GSIMP, VM1-VM2	(b) GSIMP, VM2	(c) UIM-2, VM1-VM2
C= 172.58	C=159.59	C= 157.03

Fig.2 Optimization results of the cantilever beam under a load on the right-bottom corner

It is found that UIM-2 scheme is the better choice for the structural topology optimization of multiple materials with mass constraint. This advantage of UIM-2 model might be attributed to the linearity and separability of the mass constraint in terms of design variables.

4.2 Cantilever beam under a load on the middle of right edge

As shown in Fig.3, the structure is the same with the last example, but the load location is different. In this section, only UIM-2 is adopted.
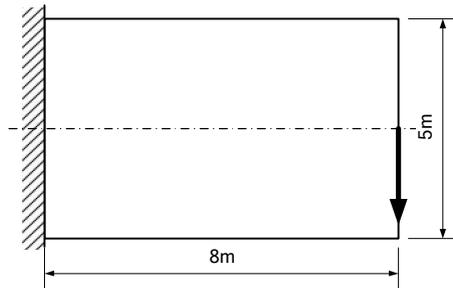

Fig.3 Cantilever beam under a load on the middle of right edge

Suppose $\overline{mass}=70\times10^3\,\mathrm{kg}$. For the optimization problem with VM3-VM1, both VM1 and VM3 are used in the optimization design, as shown in Fig.4.2(a). Comparatively, the results with single solid material (VM1 or VM3) are shown. According to the compliances of the optimization results, the design with both VM1 and VM3 is the best.
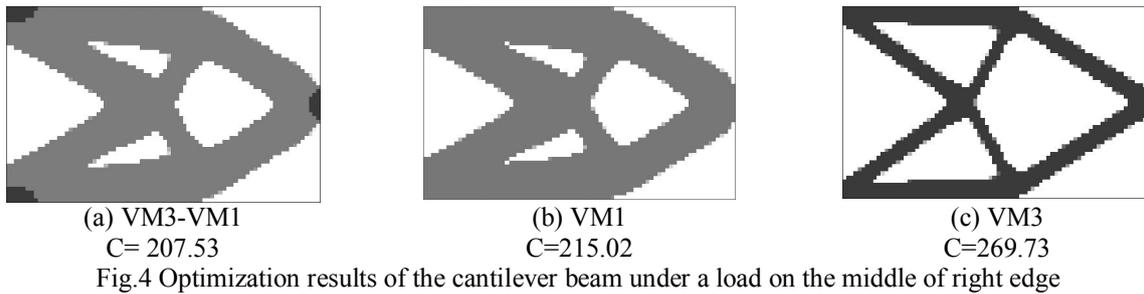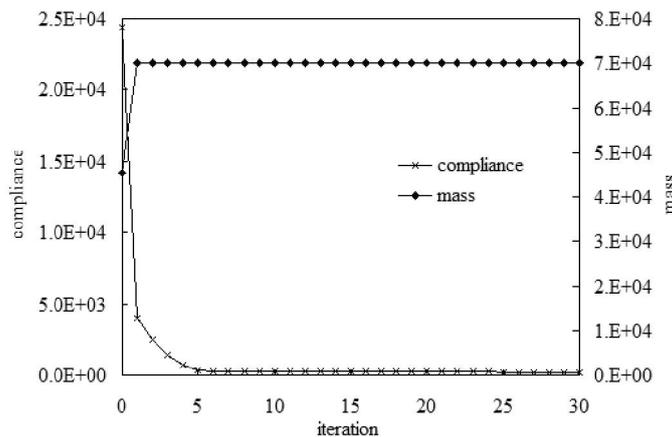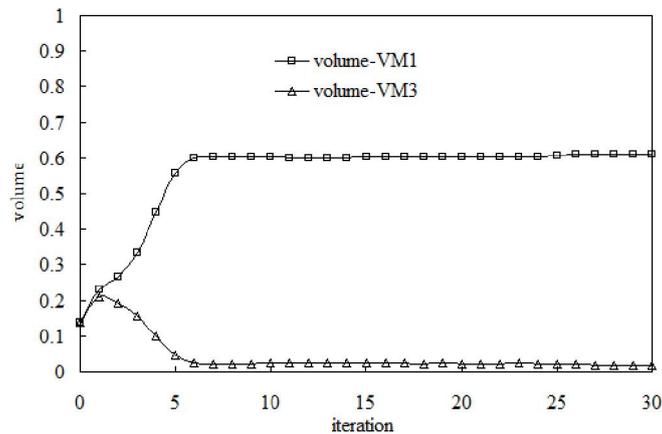

(a) VM3-VM1   (b) VM1   (c) VM3
C= 207.53   C=215.02   C=269.73

Fig.4 Optimization results of the cantilever beam under a load on the middle of right edge

The iteration histories of the design problem with VM3-VM1 are plotted in Fig.5. Obviously, the optimization iteration is very stable.

(a) Iteration history of the structural compliance and mass

(b) Iteration history of the solid material volume

Fig.5 Iteration history (VM3-VM1)

The influences of the upper bound of mass constraint upon the amount of the solid materials are shown in Fig.6. The amount of VM3 increases monotonously with the upper bound of the mass constraint. In contrast, the volume of VM1 increases firstly and then decreases. It means that the material with larger stiffness-to-mass ratio is more appropriate although its Young's modulus is smaller when the upper bound of structure mass is small. If more materials are allowable, the structure consisting of more harder materials is stiffer.
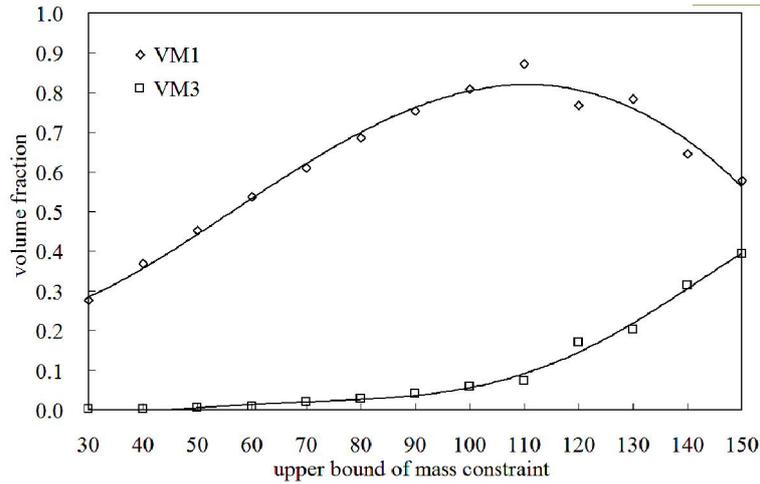
Fig.6 Influences of the mass constraint upon the volumes of the solid materials (VM3-VM1)

For the optimization problems with VM3-VM1 and VM1, the influences of the upper bound of mass constraint on the compliance of the optimization results are shown in Fig. 7. For these optimization problem, two solid materials always yield better designs.
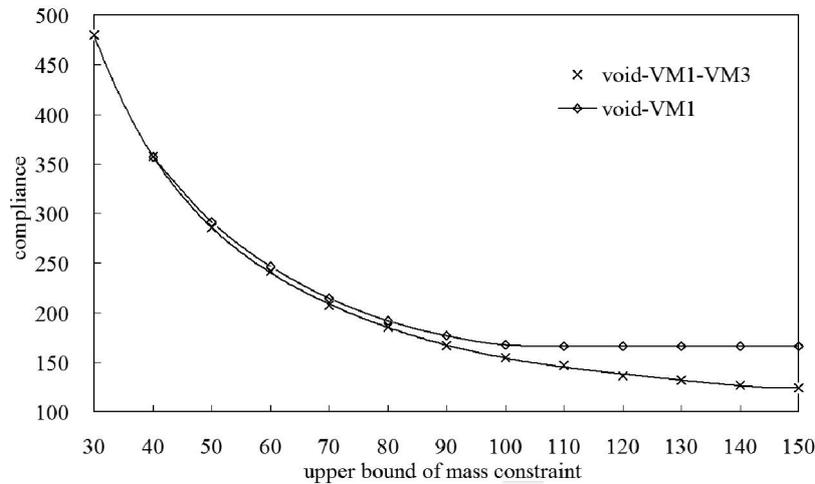

Fig.7 Influences of the mass constraint upon the compliance

A comparison between the optimization results with mass and volume constraints is made here. Suppose that the structure mass is less than $70 \times 10^3 \, \mathrm{kg}$. If the upper bound of the volume constraint of VM1 is fixed a priori, the upper bound of the volume constraint can be determined for VM3 correspondingly. The influence of the amount of VM1 on the optimization results are plotted in Fig.8. For the optimal solution with the mass constraint, the volume fractions of VM1 and VM3 are 0.6102 and 0.0190, respectively. Using these volume fractions as the upper bounds of the volume constraints, the optimal solution is very similar to that with mass constraint. Besides, this solution is better than any others with volume constraint in the sense of compliance minimization. Obviously, the mass constraint always leads to a better solution than the volume constraint with the precondition of the same structure mass. For most engineering problems, the mass constraint is more significant and important than the volume constraint to find the optimal design.
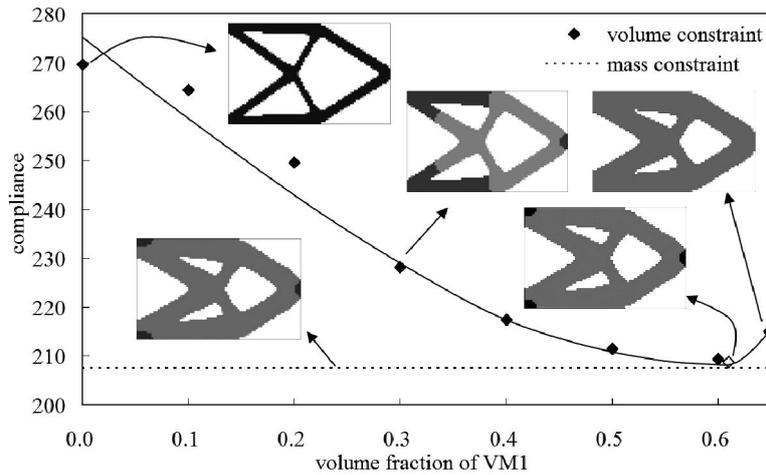
Fig.8 Comparison of the optimization results with mass and volume constraint

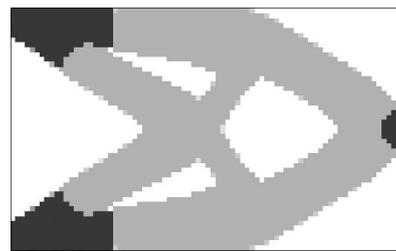4.3 Three solid materials problem

Taking the cantilever beam in Fig. 3 as an example, three solid materials (VM1, VM3 and VM4) are considered and UIM-2 scheme is adopted. Firstly, only the mass constraint is included and $\overline{M} = 70 \times 10^3 \, \text{kg}$. As shown in Fig.9(a), the optimal structure consists of VM4, namely the material with largest stiffness-to-mass ratio. If the amount of VM4 is limited, for example 10%, the optimization result is shown in Fig.9(b). The dark area is filled with VM4 and the gray area indicates VM1. When the volume constraint of VM4 is added, VM1 will play the role in the structure, while VM3 is still not chosen because its stiffness-to-mass ratio and Young's modulus are both the smallest. It is also noticed that the volume constraint of VM4 is active in this optimal solution. Besides, the additional volume constraint is a binding constraint that reduces the design space of the optimization problem so that the value of the objective function is larger than that without one such volume constraint. For both results, the structure mass attains its upper bound.

(a) mass constraint
C=110.14
VM1: 0%; VM3: 0%; VM4: 48.4%

(b) mass and volume constraint of VM4
C=164.37
VM1: 51.3%; VM3: 0%; VM4: 10.0%

Fig.11 Optimization results of the three-phase solid materials problem

5. Conclusions

For the structural topology optimization problems of multiphase materials, it is observed that the mass constraint is more significant and important than the volume constraint. GSIMP and UIM interpolation schemes are presented and compared. The mass constraint in the adopted UIM-2 scheme holds the linearity and separability in terms of design variables, while the constraint in the GSIMP scheme is nonlinear with coupling terms. From the viewpoint of solution efficiency, the former favors very much the mathematical programming approaches, especially the convex programming methods. Numerical examples indicate that the proposed UIM-2 scheme is efficient and reliable to solve the topology optimization problem with multiphase materials under the mass constraint.

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8

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