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Phase Field: A Variational Method for Structural Topology Optimization

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Abstract: In this paper we present a variational method to address the topology optimization problem – the phase transition method. A phase-field model is employed based on the phase-transition theory in the fields of mechanics and material sciences. The topology optimization is formulated as a continuous problem with the phase-field as design variables within a fixed reference domain. All regions are described in terms of the phase field which makes no distinction between the solid, void and their interface. The Van der Waals-Cahn-Hilliard theory is applied to define the variational topology optimization as a dynamic process of phase transition. The Γ-convergence theory is then adapted for an approximate solution to this free-discontinuity problem. As a result, a two-step, alternating numerical procedure is developed which treats the whole design domain simultaneously without any explicit tracking of the interface.

Within this variational framework, we show that a regularization theory can be incorporated to lead to a well-posed problem formulation. We also show that the phase-field model has a close relationship with the general Mumford-Shah model of image segmentation in computer vision. The proposed variational method is illustrated with several 2D examples that have been extensively used in the recent literature of topology optimization, especially in the homogenization based methods. Extension of the proposed method to the general problems of multiple material phases other than just solid and void is discussed, and it is further suggested that such a variational approach may represent a promising alternative to the widely-used material distribution model for the future development in topology optimization.

keyword: Topology optimization, phase field model, phase transition method, regularization method

1 Introduction

Aiming at one of the most challenging tasks in structural optimization, the field of topology optimization of continuum structures has been thriving in the past decades with a wide range of techniques having been developed (Bendsoe (1988, 1999, 2003); Bendsoe (1999); Tapp (2004); Mathur (2003); Ibrahimbegovic and Knopf-Lenoir (2003)). In contrast to the classical shape optimization problems (Bendsoe (2003); Rozvany (2001); Sokolowski (1992)), the essential concept of topology optimization is to admit changes in the connectivity of the geometry of the structure in the optimization procedure, thus increasing the potential of finding the best structural design for the specified performance requirements and design constraints. This computational problem is often referred to as the variable-topology optimization (Bendsoe (1999)).

Up to date, the dominant approach to the topology optimization is to treat the problem as a material distribution over a fixed reference domain $\Omega \subseteq R^d \quad (d = 2 \text{ or } 3)$. The optimal design A is a part of the reference domain $A \subset \Omega$ and it can be represented by its characteristic function $\chi(x) : \Omega \rightarrow \{0,\ 1\}$ such that $\chi(x) = 1$ if $x \in A$ and $\chi(x) = 0$ otherwise (Bendsoe (2003); Bendsoe (1999)). In this domain, we seek the optimal distribution of material, through specified objective and constraint functions. The physics of the problem is also defined on the fixed reference domain with a modeling and analysis tool provided. In discrete form, a "raster" geometric model is often employed with a refined finite element grid covering the reference design domain, similar to a black-and-white rendering of a digital image (Bendsoe (2003); Bendsoe (1999)). This formulation is known as the "basic" topology optimization or the "generalized" shape optimization, as the design is an unrestricted "0-1" integer design which specifies *unambiguously* either solid or void at every point in the reference domain.

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Unfortunately, the basic problem of topology optimization is an *ill-posed* problem in its mathematical theory and numerical methods (see e.g. (Haber (1996))). As first observed numerically in (Cheng (1981)) for a variable-thickness plate design problem, the optimization problem may not admit a solution. Particularly for the problem of minimizing the structural compliance of an elastic body for a specified set of loads and supports, it has been illustrated that a non-convergent design sequence can be constructed such that the compliance reduces monotonically (Bendsoe (2003)). The resulting design has a configuration with an unbounded number of microscopic holes, rather than a finite number of macroscopic holes.

Well-posed problems can be generated by a relaxation or regularization procedure by allowing homogenization of the properties of the material (Bendsoe (2003)). Relaxation usually yields continuous design variables over the reference domain, similar to the grey-scale rendering of an image, and it circumvents the numerical difficulties associated with the discrete "0-1" formulation. However, it is no longer possible to unambiguously define a point of either solid or void from the homogenized solution. Perforated microstructures are also difficult to manufacture. Thus, the "relaxed" optimal solutions may not lead directly to useful and practical designs.

Another regularization method is the explicit penalization of intermediate values of the material density. The suppression technique becomes quite popular, especially with the "solid isotropic material with penalization" (SIMP) approach for its conceptual and practical simplicity (Bendsoe (2003); Rozvany (2001); Sigmund (1998)). It has been pointed out that certain penalties on intermediate densities can be interpreted in physical terms as equivalent to restrictions on the micro-structural configuration (Bendsoe (1999)). With this computational strategy, various suppression-based regularization approaches have been suggested, including adding more constraints into the problem such as perimeter controls (Petersson (1999)) and slope constraints (Diaz (1995); Sigmund (1998)), and employing filters for chattering solutions (Bourdin (2001); Sigmund (2000); Sigmund (1998)), and they have been widely applied to problems with multiple physics and multiple materials (Bendsoe (2003); Bendsoe (1999); Rozvany (2001); Sigmund (2000)). Fundamentally, however, the suppressions do not directly address the chattering problem underlying the relaxation concept.

In a recent overview of the field by Bendsoe (Bendsoe (1999)), it is concluded that the approach of material distribution in the fixed domain offers many beneficial features particularly in terms of computational efficiency. This is evident from the successful applications of the methods in industry. It is also pointed out incisively that the approach has some intrinsic features that are less desirable. The chief one is the dependency of the design variables of material density on the finite element grid. This dependency yields a number of drawbacks, including a lack of an unambiguous mapping from the model to design, under-resolved finite element solutions for the physical response, and spurious numerical behavior caused by the coupling with finite element models. These fundamental issues are often argued in the literature (Ruiter (2000)) from investigations into alternative approaches such as the evolutionary approaches (Reynolds (1999); Xie (1993); Tapp (2004); Mathur (2003)), material interpolation (Ruiter (2000); Yin (2001)), and the level-set methods being developed more recently (Wang (2003); Wang (2003); Wang and Wang (2004); Sheen (2003)).

In this paper we present a variational method – *phase transition* – to address the topology optimization problem. Similar to the setting of material distribution approach, the design is restricted within a fixed reference domain. A continuous variable $\rho(x)$ is used within the design domain $x \in \Omega$ such that the characteristic function of the structure being designed is defined by $\chi(x) : \Omega \rightarrow [0,\ 1]$. However, in contrast to the use of homogenized or penalized material properties, the model of material properties is isotropic and linear with respect to the design variable $\rho(x)$, such as $\rho(x)$ resembles the material density in the case of a single material structure. As in the basic topology optimization problem, this problem is also ill-posed. Therefore, we will apply a regularization theory to lead to a well-posed problem formulation. This is to be accomplished with a variational model, without the use of material homogenization or material interpolation (or penalization). The basic idea of regularization is the same as in the homogenization-based methods (or the SIMP methods) – It is to impose some constraints on the solution $\rho(x)$ so the space of admissible solutions is restricted. For instance, a regularization may be chosen to induce a smooth solution or a solution preserving sharp transitions of the variable $\rho(x)$ across x (known as an "edge-preserving" solution).

In addition to the regularization, we will employ another variational model devoted to obtain a "region segmentation" of the reference domain. The goal is to result in a black-and-white design with optimal physical performance. The role of this variational model is to partition the reference domain into distinct regions, each region being characterized by the feature of being either solid $(\rho(x) = 1)$ or void $(\rho(x) = 0)$. Hence, the final solution will be made of homogeneous solid or void regions separated by sharp regularized boundaries.

To achieve this goal, we adapt the *theory of phase transitions* from mechanics and material sciences, where the problem of stability of systems containing several instable components has been extensively studied over years. These components may be liquid phases having different levels of density distribution (Allen (1979); Cahn (1958)) or solid phases under solidification (Warren (1995)). Through the Van der Waals-Cahn-Hilliard theory of phase transitions, the stable configuration is proven to be a compound of homogeneous regions separated by sharp interfaces having minimal length. The theory also leads to the analysis of the interface between the phases during the process of phase transition to the system stability. In our variational approach proposed here, we formulate the topology optimization problem as a phase transition problem and apply these mechanics results to form a framework of variational topology optimization.

Our work presented here is also inspired by recent developments in digital image processing with variational methods. In particular, variational models incorporating the theory of phase transitions have been successfully applied in the field of image classification (March (1992); Samson (2000)), where a given digital image has to be segmented into different areas characterized by parameters associated with the spatial distribution of image intensity, color, or texture, often along with an image restoration and edge regularization. Our variational model bears many similarities with variational image segmentation models; however, our process of optimization might be regarded as an inverse process of image classification. In an application to problems of design-dependent loads, the phase-field model is used for topology optimization independently (Bourdin (2003)), where some theoretical proofs of convergence are given.

In the following, we first define the variational problem of topology optimization. A *phase-field* model is described for diffusion-based regularization and phase transition. We then recall the Van der Waals-Cahn-Hilliard theory of phase transitions in mechanics. We show how the interface between different phases can be represented by the phase-field model as a *diffuse-interface* (or "soft"-interface) without resorting to explicit interface tracking. This phase-filed model is further examined for its relationship with the Mumford-Shah model widely used in image segmentation. We then discuss a method of numerical solution to the variational problem based on the theory of Γ-*convergence* in the field of free-discontinuity problems. We present a numerical algorithm for the topology optimization. Finally, the proposed variational method is illustrated with three 2D examples of mean compliance minimization typically used in the literature of topology optimization, especially in the homogenization based methods.

2 The Variational Topology Optimization Problem

In this paper we use a linear elastic structure to describe the problem of structural optimization. Conceptually, the approach presented here would apply to a general structure model. Let $\Omega \subseteq R^d \quad (d = 2 \text{ or} 3)$ be an open and bounded set occupied by a linear isotropic elastic structure. The boundary of Ω consists of three parts: $\Gamma = \partial\Omega = \Gamma_0 \cup \Gamma_1 \cup \Gamma_2$, with Dirichlet boundary conditions on Γ_1 and Neumann boundary conditions on Γ_2. It is assumed that the boundary segment Γ_0 is traction free. The displacement field u in Ω is the unique solution of the linear elastic system

$$\begin{aligned} -\operatorname{div}\sigma(u) &= f && \text{in } \Omega \\ u &= u_0 && \text{on } \Gamma_1 \\ \sigma(u)\cdot n &= h && \text{on } \Gamma_2 \end{aligned} \tag{1}$$

where the strain tensor ε and the stress tensor σ at any point $x \in \Omega$ are given in the usual form as

$$\varepsilon(u) = \frac{1}{2}\left(\nabla u + \nabla u^T\right) \qquad \sigma(u) = E\varepsilon(u) \tag{2}$$

with E as the elasticity tensor, u_0 the prescribed displacement on Γ_1, f the applied body force, h the boundary traction force applied on Γ_2 such as an external pressure load exerted by a fluid, and n the outward normal to the boundary.

2.1 The Basic Topology Optimization Problem

The "basic" problem of structure optimization is specified with respect to a specific objective function described by $F(u)$ such that

$$\begin{aligned} &\underset{\Omega}{\text{minimize}} && J(u,\Omega) = \int_\Omega F(u)\, d\Omega \\ &\text{subject to}: && G(u,\Omega) \le 0 \end{aligned} \tag{3}$$

The variational equation of the linear elastic equilibrium is written as

$$\begin{aligned} &\int_\Omega E\varepsilon(u) : \varepsilon(v)\, d\Omega \\ &= \int_\Omega f \cdot v d\Omega + \int_{\Gamma_2} h \cdot v d\Gamma, \text{ for all } v \in U \\ &U = \left\{u :\ u \in H^1(\Omega); u = u_0 \text{ on } \Gamma_1\right\} \end{aligned} \tag{4}$$

with U denoting the space of kinematically admissible displacement fields and ':' representing the second order tensor operator. The system constraints are described by function $G(u,\Omega)$, including, for example, the limit on the amount of material in terms of the maximum admissible volume of the design. The goal of optimization is to find a minimizer Ω.

In this standard black-and-white notion of structural optimization, the characteristic function of the design is given as (Bendsoe (1988, 2003); Bendsoe (1999)):

$$\chi(x) :\ \Omega \to \{0, 1\} \text{ such that}$$
$$\chi(x) = \begin{cases} 1 & \text{for } x \in A \\ 0 & \text{for } x \in \Omega\backslash A \end{cases}$$

with the solid part of Ω being occupied by A. The elasticity tensor in Ω is given by $E(x) = \chi(x) E^0$ in terms of rigidity E^0 of the given material.

A popular technique to amend the discrete optimization problem is to consider a reformulation of the problem in terms of continuous variables,

$$\rho(x) : \Omega \to [0,\ 1] \quad \text{and} \quad E(x) = \rho(x) E^0 \tag{5}$$

for the elasticity tensor in Ω. We have solid material where $\rho = 1$ and void wherever $\rho = 0$. Intermediate values of ρ indicate "transitional" material between solid and void. In the continuous formulation, there is generally no particular physical significance to the transitional material; it is solely for providing a continuous problem formulation. In the final solution, variable $\rho(x)$ should take an extreme value of either 1 or 0. This is usually accomplished with a penalty term to suppress transitional material in the optimal design. This requirement may lead to a model of material interpolation (e.g., the SIMP model) with a natural physical relevance (Bendsoe (1999); Gibson (1997)).

The discrete and the continuous problem as stated with no additional geometric constraints are known to be ill-posed. As discussed in Introduction section, the homogenization method has been a key idea in most of the earlier work on making the problem well-posed. Another regularization technique is to introduce additional constraints on the solution such as perimeter or slop constraints (Jog (2002); Sigmund (1998)). Here, we shall introduce a variational model based on the regularization theory in image processing and the phase-transition theory in mechanics.

2.2 Variational Models of the Optimization

A classical method to overcome an ill-posed problem is to add a regularization term to the objective function. This is a widely used method in the field of image processing. For instance, a smoothing term $\int_\Omega |\nabla\rho|^2 dx$ can be introduced in J as Thikonov regularization (Tikhonov (1997)). This is known as isotropic smoothing in the field of variational approaches (Mumford (1989); Samson (2000)).

Thikonov regularization is equivalent to linear (Gauss) filtering of the solution field. It is well known in the field of image processing for its strong isotropic smoothing properties, but it does not preserve edges. In our topology optimization problem, "edges" would represent the boundary of the structure. Boundaries are the most important features in our problem, and they are defined as *sharp* transitions of the density level. Thus, the regularization method should be able to yield sharp material transitions, or "edge-preserving".

Following the variational analyses of anisotropic smoothing developed in the field of image processing (Chambolle (1995); Charbonnier (1997)), we introduce a common regularization model for the continuous topology optimization problem with the following optimization functional

$$J(u,\rho) = \int_\Omega F(u,\rho) dx + \mu \int_\Omega \varphi(|\nabla\rho(x)|)\, dx \qquad (\mu > 0)$$

(6)

Function φ is regular and continuously differentiable. In order to achieve an "edge"-preserving effect, φ should be chosen to have at least the three following properties (Charbonnier (1997); Samson (2000)):

1. $\varphi'(s)/s$ is strictly decreasing on $s \in [0, \ \infty\}$.
2. $\varphi'(0) = 0, \ \lim\limits_{s \to 0} \varphi'(s)/s = \varphi''(0) = \beta$, and $0 < \beta < \infty$.
3. $\lim\limits_{s \to \infty} \varphi'(s)/s = \lim\limits_{s \to \infty} \varphi''(s) = 0$.

The first property is for avoiding numerical instabilities. The second condition requires $\varphi(s)$ to be quadratic or nearly quadratic for $s \to 0$, and it is for the regularization effect of smoothing where variations of the density are weak. The third condition requires $\varphi(s)$ to be linear or sub-linear for $s \to \infty$. This is for the edge-preserving effect, where in a neighborhood of the boundary the density presents a strong gradient. It is preferable to diffuse the density along the tangent direction of the boundary and not across it. Such a typical function is $\varphi(s) = s^2/\left(1+s^2\right)$ and its behavior is illustrated in Fig. 1, together with some other commonly used functions.

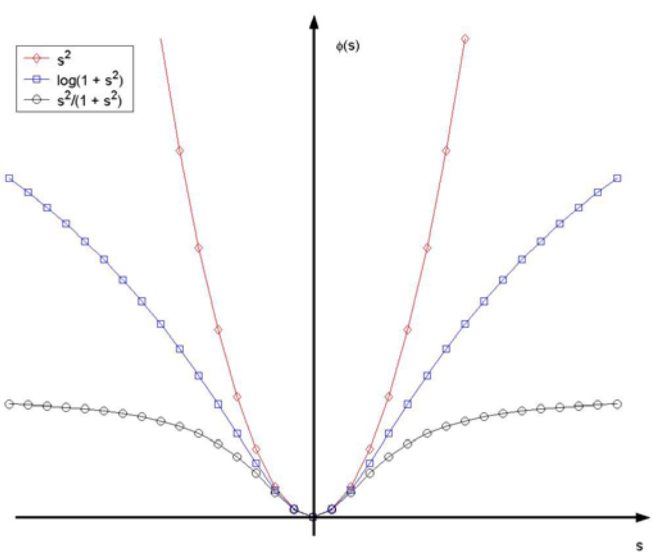

Figure 1 : Behavior of some regularization functions.

The function $\varphi(s)$ may be convex or non-convex. When φ is convex, a theoretical study about the minimizers for J can be established, such as for their existence and uniqueness. On the other hand, it is often difficult for such a theoretical study for a non-convex function φ. Nevertheless, non-convex functions are found to work well or even to provide better results in image restoration and classification (Chambolle (1995); Charbonnier (1997)). Some widely used edge-preserving φ functions include $\varphi(s) = |s|$ (total variation), $\varphi(s) = s^2/\left(1+s^2\right)$, and $\varphi(s) = \log\left(1+s^2\right)$, to name a few.

The above two properties imposed on the regularization function φ are highly qualitative. Naturally, they are not sufficient to ensure that the transitional density $0 < \rho < 1$ in the optimal design will be suppressed. This is often accomplished by introducing an explicit penalty on intermediate density values (e.g., the "power-law" in the SIMP method) or by manipulating the material model to obtain an implicit penalty. These are popular methods used in most of the work on topology optimization, especially with the homogenization and the SIMP methods (Bendsoe (2003); Rozvany (2001); Sigmund (2000)).

Here, we take a direct view of the issue and consider the topology problem of the structure as a *region segmentation* problem. This means that the optimization process remains to produce a black-and-white design, where the whole material domain of the structure will be partitioned into distinct regions of solid or void phase, and every point of a partitioned region belongs to the same "phase class" of solid or void. In other words, for every point $x \in \Omega$ we must be able to determine if x is a boundary point on an interface between regions and which material phase (i.e., solid or void) it belongs to.

For this "segmentation" purpose, we need to modify our variational model as follows:

$$J(u,\rho) = \int_\Omega F(u,\rho)dx + \mu \int_\Omega \varphi(|\nabla\rho(x)|)\,dx + \eta \int_\Omega W(\rho(x))dx \tag{7}$$

Here, the additional term W is a potential inducing a "region classification" constraint. It takes into account the density ρ of the material phase classes (i.e., solid and void) for the classification of each point x. It has as many minima as the number of phases (i.e., 2 in the black-and-white case) and imposes a level constraint on the solution. The positive parameters $\mu > 0$ and $\eta > 0$ are the weights in the variational model. This is a model adapted from the phase-field theory of phase transition problems studied in mechanics.

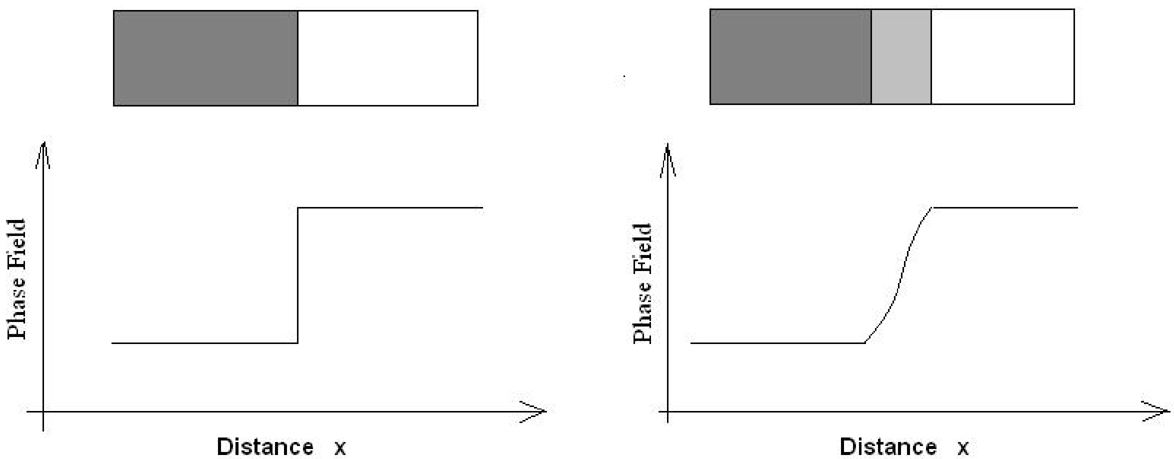

Figure 2 : The sharp interface (left) and the diffuse interface (right)

3 The Phase-Field Model

The theory of phase transitions has been developed for the study of mechanical systems of a material compound of instable phases (Allen (1979); Cahn (1958); Eyre (1993)). The material may be solid or liquid of two of more phases. The common problem is to characterize the stability of such a system and to describe the interface between the phases while the system undergoes a physical process (e.g., solidification) to reach its stability. From this process point of view, there is a similarity between our basic topology optimization problem (3) and a phase transition system of two material phases.

In an unstable configuration of a two phase mixture, there are three distinct quantities to consider: the two distinct material phases and their interface. The interface can be described as an evolving surface whose motion is controlled according to the physical models consistent with the mechanism of transformation. The interface is simply a mathematical surface with no width or structure; it is said to be a *sharp-interface*. The phase interface, however, may have a complex topology, and the need to track this boundary has made sharp-interface models difficult to use and to implement with good numerical properties. These difficulties associated with topological changes in the problems of phase transitions such as alloy solidification are essentially identical to those of the problem of topology optimization.

In recent years, an alternative to the sharp-interface model – the *phase-field* method – has emerged in the fields of mechanics and material sciences. In the phase-field method, the state of the entire multi-phase system is represented continuously by a single variable f known as the *field parameter* in thermodynamics. For example, $f = 1$, $f = 0$, and $0 < f < 1$ represent the two distinct phases of solid and fluid and the interface respectively. The interface is therefore located by the region over which f changes from, for example, the liquid phase to the solid phase. The range over which it changes is the width of the interface. Therefore, the interface is also regarded as a *diffuse-interface*, as illustrated in Fig. 2. The set of values of the parameter over the whole system domain is the *phase field*. Such a phase-field model eliminates the assumption of a sharp interface and the concomitant need to track its motion. Indeed, if a theory can be created to describe the dynamics of transitions between the phases in terms of the field parameter, then we no longer need to track the interface. Instead we can follow the evolution of the phase field.

It is straightforward to adapt such a phase field model for solving our variational topology problem (7). For the sake of clarity, we concentrate our discussion on the case of single material structures, i.e., of two phases of solid and void. Our phase field parameter is simply made as $\rho = f$, while $\rho = 1$ representing solid and $\rho = 0$ the void. Then, the intermediate values of ρ $(0 < \rho < 1)$ have a new meaning – they indicate the interface between solid and void or the boundary of the structure being optimized. For this adapted phase field model, the Van der Waals-Cahn-Hilliard theory of phase transitions is the most relevant theory to use.

3.1 The Theory of Phase Transitions

Strategically, what we need to describe our variational approach with a phase-field model is to define an optimization process with the phase-field variables $\rho(x)$ in our system. In particular, we must first formulate the dynamics of the phase transition. The dynamic model we consider is based on the phase transition theory of Van der Waals and Cahn-Hilliard in mechanics (cf. (Allen (1979); Cahn (1958); Eyre (1993); Leo (1998)).

The evolution of a two-phase mechanical system is assume to be governed by a generalized free energy in the following form

$$E(\rho,\varepsilon) = \varepsilon \int_{\Omega} |\nabla \rho(x)|^2 dx + \frac{1}{\varepsilon} \int_{\Omega} W(\rho(x)) dx \qquad (8)$$

The first term in E depends only on the gradient of $\rho(x)$ and hence is non-zero only in the interfacial region. Thus, it represents the interfacial energy of the system and it acts to stabilize the interfacial transition region. The second term, as in the classical Cahn-Hilliard theory (Eyre (1993)), is taken to be a double-welled potential so that the system separates into two distinct phases of $\rho = 1$ (solid phase) and $\rho = 0$ (void phase) such that $W(1) = W(0) = 0$. Furthermore, it is assumed that W is quadratic around $\rho = 1$ and $\rho = 0$ and is growing at least linearly at infinity. The presence of the coefficient ε is necessary in order for the diffuse-interface system to converge to the sharp-interface system, in the limit as $\varepsilon \to 0$. These two generalized free energy terms together keep the thickness of the interfacial region proportional to ε.

3.2 The Γ-convergence Technique

The Van der Waals-Cahn-Hilliard theory has let to the introduction of the perturbation term $\varepsilon|\nabla\rho|^2$, with small ε. The asymptotic behavior of the model as $\varepsilon \to 0$ allows us to solve for stable configurations characterized by

$$\min_{\rho} \left\{ \int_{\Omega} W(\rho(x)) dx,\ \rho\colon \Omega \to [0\ \ 1],\ \int_{\Omega} \rho(x)\, dx = M \right\}$$

where M is the total mass of the material phases. This technique belongs to the general theory of Γ-convergence, and it has been extensively studied as the subject of gradient theory of phase transitions (Braides (2002)). The numerical analyses for the variational problem of minimizing (8) concern a sequence of minimizers of $E(\varepsilon,\rho)$ as $\varepsilon \to 0$ (Braides (2002); Charbonnier (1997)). Γ-convergence implies existence of a minimum solution and the convergence of the minimizer sequence to the minimum solution (Braides (2002)).

When $\varepsilon \to 0$ it can be seen that the contributions of the two integral terms in E of (8) have the same order for the minimizing sequence. The role of the term W is clear: It forces the stable solution to take one of the two phase field values 1 and 0, while the effect of the gradient energy $|\nabla\rho|^2$ term is to penalize unnecessary interfaces. In fact, it is proven that the Γ-convergence sequence results in a *minimal perimeter* of the interface between the two phases (Braides (2002)). Thus, the generalized free energy has a regularization effect on the solution $\rho(x)$ by avoiding formation of any singularities and by restricting the space of solutions. While problem (8) involves only smooth functions for diffuse-interface, its counterpart of the limit sequence gets involved with only discontinuous functions for sharp-interface. The Van der Waals-Cahn-Hilliard theory of phase transitions provides a well-founded framework for solving our variational topology optimization problem (7).

3.3 The Phase-Field Model

Based on the previous sections on model regularization (Section 2.1) and on the phase transition theory (Section 3.1), it is straightforward to transport these ideas into a computational model for the continuous variational topology optimization (7). The phase-field model relies on the minimization of the following generalized "energy" function

$$\begin{aligned} J_{\varepsilon}(\rho,u) = &\int_{\Omega} F(u)\, dx + \varepsilon\mu \int_{\Omega} \varphi(|\nabla\rho(x)|)\, dx \\ &+ \frac{\eta}{\varepsilon} \int_{\Omega} W(\rho(x)) dx \end{aligned} \qquad (9)$$

The corresponding topology optimization problem is to find a solution ρ^* such that

$$\rho^* = \lim_{\varepsilon \to 0} \left[\arg \min_{\rho} J_{\varepsilon}(\rho,u) \right] \qquad (10)$$

subject to all given constraints.

As before in (7), $\varphi(s)$ might be taken as an edge-preserving function. When φ is a convex function, the inclusion of the objective functional $\int_{\Omega} F(u)\, dx$ has no effect on the conclusions of the Γ-convergence theory stated before (Braides (2002); Samson (2000)). Thus, as

$\varepsilon \to 0$ there exists a sequence of minimizers ρ of J_ε converging to a solution of distinct regions of solid and void separated by sharp interface with regularized properties, i.e., of minimal length in perimeter. When ε is not too small ($\varepsilon >> 0$), the level constraint of the third term of J_ε is quite insignificant; only smoothing process occurs with the second term. As ε further decreases, the diffusion process gets progressively "softened", while the "classification" process get stronger in the third term. This would "sharpen" the interface and force the solutions to form distinct phase regions. While the mathematical analysis is yet to complete for a general objective function $F(u)$ rather than the structure's mean compliance, various numerical experiences seem to confirm that the variational formulation provides a well-behaved framework for seeking meaningful optimal solutions, particularly when the models of the structure have finite perimeter.

3.4 Relation to the Mumford-Shah Model

It is interesting to examine the relationship of the phase-field model with the problem of segmentation in image processing and computer vision. This provides a different perspective of our variational approach proposed here. The most celebrated criterion for image segmentation is the model introduced in (Mumford and Shah (1989)). In the model, an image is decomposed into a set of regions within the bounded open set Ω. These regions are separated by a set of smooth "edges" B. The image segmentation problem is formulated as a variational problem to minimize the following functional

$$J_{MS}(f,B) = \int_\Omega I(f)\,dx + \alpha \int_{\Omega\backslash B} |\nabla f(x)|^2\,dx + \beta \int_B dS \tag{11}$$

where $I(f)$ is an image restoration model (e.g., the least squares model) for an meaningful image processing. The second term, with $\alpha > 0$, provides an optimal piecewise smoothing within each segmented region, while the third term leads to boundaries of minimal perimeter ($\beta > 0$). Since B represents a set of variables of free discontinuities, the perimeter $\int_B dS$ must be defined as the one-dimensional-less Hausdroff measure of B (Chambolle (1995); Mumford (1989)). For a piecewise homogeneous image, the expected solution is piecewise constant. The minimization of J_{MS} is a free discontinuity problem and is a difficult problem to solve (Ambrosio (1990); Bourdin (2000); Mumford (1989)). In the framework of Γ-convergence, the perimeter energy in the Mumford-Shah model can be approximated by a quadratic integral of an edge signature function $z(x)$ such that

$$\int_B dS = \int_\Omega \left(\varepsilon |\nabla z|^2 + \frac{1}{4\varepsilon}(z-1)^2 \right) dx, \;\; \varepsilon << 1 \tag{12}$$

as proposed in (Ambrosio (1990)). This approximation leads a sequence of functions as $\varepsilon \to 0$ to converge to the Mumford-Shah functional, thus yielding an approximate solution to the free discontinuity problem. Clearly, the edges in the image are represented by a set of diffuse interfaces as opposed to sharp ones. This approximation process of image segmentation can be viewed with a physical interpretation involving the model of phase transitions described in Section 3.1.

Conversely, we may view our problem (3) of the topology optimization of structures in a broader perspective of the Mumford-Shah type framework: The optimal structure has a meaningful boundary set Γ which leads to a complete partition of the design domain Ω such that $\Omega = \cup_i \Omega_i \cup \Gamma$, and each connected component Ω_i of $\Omega\backslash\Gamma$ represents one physical component of the structure with a unique physical and material feature (such as of distinct isotropic or anisotropic properties). A variational model that appropriately combines the effects of both the boundary set Γ and its separated regions $\{\Omega_i,\ i = 1,2,\cdots\}$ could be described as, similarly to the Mumford-Shah model,

$$J_{MS}(f,\Gamma) = \int_\Omega F(f)\,dx + \alpha \int_{\Omega\backslash\Gamma} \varphi(|\nabla f(x)|)\,dx + \beta \int_\Gamma dS \tag{13}$$

4 Minimization Algorithms

Based on the previous discussions, we now define the general objective functional of our variational model as follows:

$$L_\varepsilon(\rho,u) = \int_\Omega F(u)\,dx + \varepsilon\mu \int_\Omega \varphi(|\nabla\rho(x)|)\,dx + \frac{\eta}{\varepsilon}\int_\Omega W(\rho(x))dx + \lambda^T G \tag{14}$$

where Lagrange multipliers λ are used to incorporate the given constraint functions G, without loss of generality. The elastic displacement field u must satisfy

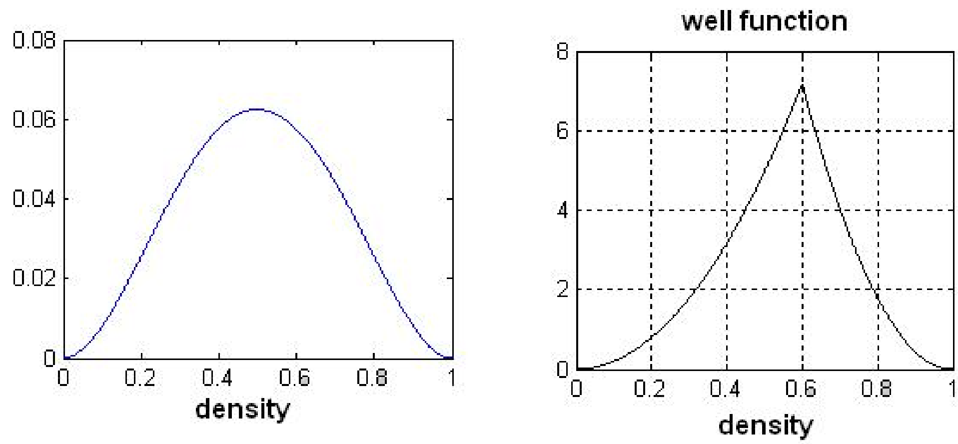

Figure 3 : Commonly used potential-well functions, continuous (left) and piece-wise quadratic (right), for $0 \leq \rho \leq 1$

the bi-linear equation (4) of the linear elasticity system. The phase-field variables ρ are defined within the range $\rho(x) \in [0\ \ 1]$. The corresponding topology optimization problem is to find a solution ρ^* such that

$$\rho^* = \lim_{\varepsilon \to 0} \left[\arg \min_{\rho} L_\varepsilon(\rho, u) \right] \tag{15}$$

and a set of Lagrange multipliers satisfying the Kuhn-Tucker conditions associated with the objective functional L_ε.

4.1 The Potential-Well Function W

Before constructing numerical algorithms, we shall discuss properties of the potential-well function $W(f)$. The phase-transition theory requires that W is quadratic around its minima and is growing faster than linearly at infinity. For each distinct phase f_i (i.e., solid and void in our case), there is a distinct minimum of W such that $W(f_i) = 0$.

For a black-and-white design problem, one may use the following double-well function

$$W(f) = f^2 (1-f)^2 \tag{16}$$

One may also use piecewise parabolic functions $W_i(f) = A_i (f - f_i)^2$ such that potential-well is quadratic around each phase value f_i and with continuous junctions as shown in Fig. 3.

4.2 Numerical Algorithm

We shall describe the numerical algorithm adapted to minimize (14). For a minimizer, the necessary condition required is the Kuhn-Tucker condition, which is derived from the Euler-Lagrange equation to compute the derivative of the functional L_ε with respect to ρ. This leads to the following system:

$$\begin{cases} F'(u) - \varepsilon\mu \,\mathrm{div}\left[\frac{\varphi'(|\nabla\rho|)}{|\nabla\rho|}\nabla\rho\right] + \frac{\eta}{\varepsilon} W'(\rho(x)) \\ +\lambda^T G' = 0 \qquad\qquad \text{for} \quad x \in \Omega \\ \\ \frac{\partial\rho(x)}{\partial n^+} = \nabla\rho \cdot n^+ = 0 \quad \text{on} \quad \partial\Omega \end{cases} \tag{17}$$

where n^+ is the outward normal to the boundary of the reference domain Ω, $div = \nabla\cdot$ denotes the divergence operator, and $F'(u)$ denotes the Euler derivative of the objective function F with respect to the phase-field variable ρ. It should be pointed out that generally F may not depend explicitly on the phase field ρ but rather on the equilibrium displacement u associated with the design. Thus, the Euler derivative may be obtained by using the general shape derivative theory. The theory has been well established (see (Haug (1986); Sokolowski (1992))), and the shape derivatives are also described in the recent work on level set methods for topology optimization (Wang (2003); Wang and Wang (2004)). We shall omit the details of its derivation here.

A straightforward way for a solution ρ seems to directly solve the partial differential equation (17). In deed, this is the method often used in a variational approach to image restoration and/or segmentation in the field of image processing, where the PDE system is linear when the Tikhonov regularization $\varphi(|\nabla\rho|) = |\nabla\rho|^2$ is used, inducing the Laplacian operator $div(\nabla\rho) = \Delta\rho$. For our problem of topology optimization, the Euler-Lagrange equations are generally nonlinear, owning to a complex Euler derivative of $F'(u)$ and/or an edge-preserving regularization function $\varphi(s)$.

Through Γ-convergence, we adopt to use a more suitable numerical scheme called the *half-quadratic regularization* (Charbonnier (1997); Samson (2000)), permitting to simplify the minimization of L_ε with reduced level of non-linearity for a fixed $\varepsilon > 0$. The basic idea of this scheme is to introduce an auxiliary variable b such that

$$\varphi(s) = \min_b \left(bs^2 + \psi(b)\right) \tag{18}$$

with the function ψ being derived from φ as $\psi(b) = g\left(\left(g'\right)^{-1}(b)\right) - b\left(g'\right)^{-1}(b)$ with $g(s) = \varphi(\sqrt{s})$ (see (Charbonnier (1997); Samson (2000)) for more details). Here, $b = \varphi'(s)/2s$, and function ψ is always convex. According to the half-quadratic algorithm, we get

$$L_\varepsilon(\rho, u) = \min_b L_\varepsilon^*(\rho, b, u) \tag{19}$$

with the "extended energy"

$$L_\varepsilon^*(\rho, b, u) = \int_\Omega F(u)\,dx + \varepsilon\mu \int_\Omega \left[b(x)\left|\nabla\rho(x)\right|^2 + \psi(b(x))\right]dx + \frac{\eta}{\varepsilon}\int_\Omega W(\rho(x))dx + \lambda^T G \tag{20}$$

$L_\varepsilon^*(\rho, b, u)$ is convex with respect to b when ρ is fixed. Thus, the extended energy $L_\varepsilon^*(\rho, b, u)$ can be minimized with respect to b in an efficient fashion. While $L_\varepsilon^*(\rho, b, u)$ is not convex in the combined variables b and ρ, we now have a two-step, alternating semi-quadratic algorithm for the minimization of $L_\varepsilon(\rho, u)$, operated through Γ-convergence as $\varepsilon \to 0$ (Braides (2002)), described as follows:

1. *Initialize variables* $\rho(x)$ *and* $b(x)$ *for* $x \in \Omega$ *and set* $i = 1$ *and* $1 > \varepsilon > 0$
2. *Repeat the following until convergence on* ρ :

   a. *Find* $b(x) = \frac{\varphi'(|\nabla\rho(x)|)}{2|\nabla\rho(x)|}$, *directly resulting from* $\min_b L_\varepsilon^*(\rho, b, u)$ *with* ρ *fixed*

   b. *Solve for* ρ *by* $\min_\rho L_\varepsilon^*(\rho, b, u)$ *with* b *fixed*

3. *Set* $i = i + 1$, *decrease* $\varepsilon\,(e.g., \varepsilon = \varepsilon^i)$, *and repeat Step 2 until* $\varepsilon \to 0$

Here, the problem of $\min_\rho L_\varepsilon^*(\rho, b, u)$ with b fixed may be solved with any of the optimization methods that have been widely used in the field of structural optimization, such as the method of moving asymptotes, the Optimality Criteria method with only a single constraint present, or a mathematical programming method (Bendsoe (2003); Rozvany (1988)).

5 Numerical Examples

Numerical examples are presented in this section for mean compliance optimization problems that have been widely studied in the relevant literature (e.g., (Bendsoe (2003); Rozvany (2001))). The objective function of the problem is the strain energy of the structure with a constraint on the material volume M,

$$J(u, \Omega) = \int_\Omega E\varepsilon(u) : \varepsilon(u)d\Omega$$
$$G(\rho) = \int_\Omega \rho(x)\,dx - M = 0 \tag{21}$$

For all examples, the material used is steel with a modulus of elasticity of 200 GPa and a Poisson's ratio of $\nu = 0.3$. For clarity in presentation, the examples are in 2D under plane stress condition. Since only a single constraint is involved in the problem, the optimality criteria method is employed in the phase-field algorithm, which is known for its simplicity and efficiency (Bendsoe (2003)).

5.1 Bridge-Type Structures

A bridge-type structure is considered first. A rectangular design domain of L long and H high with a ratio of $L : H = 12 : 6$ is loaded vertically at its bottom with multiple loads $P_1 = 40N$ and $P_2 = 20N$ as shown in Fig. 4. The left bottom corner of the beam is fixed, while it is simply supported at the right bottom corner. The volume ratio of 0.30 is considered. A mesh of 60×30 quadrilateral elements are used for the discrete analysis and optimization. A selective set of intermediate results are shown in Fig. 4, as the sequence of optimal solutions converge to the final design as $\varepsilon \to 0$. Changes in mean compliance, the regularization and the total energy terms during the convergence are shown in Fig. 5. In this example, the Thikonov regularization function $\varphi(s) = s^2$ is used. For the same problem, a finer mesh of 100×50 elements are used next, and the intermediate results and the final design are shown in Fig. 6.

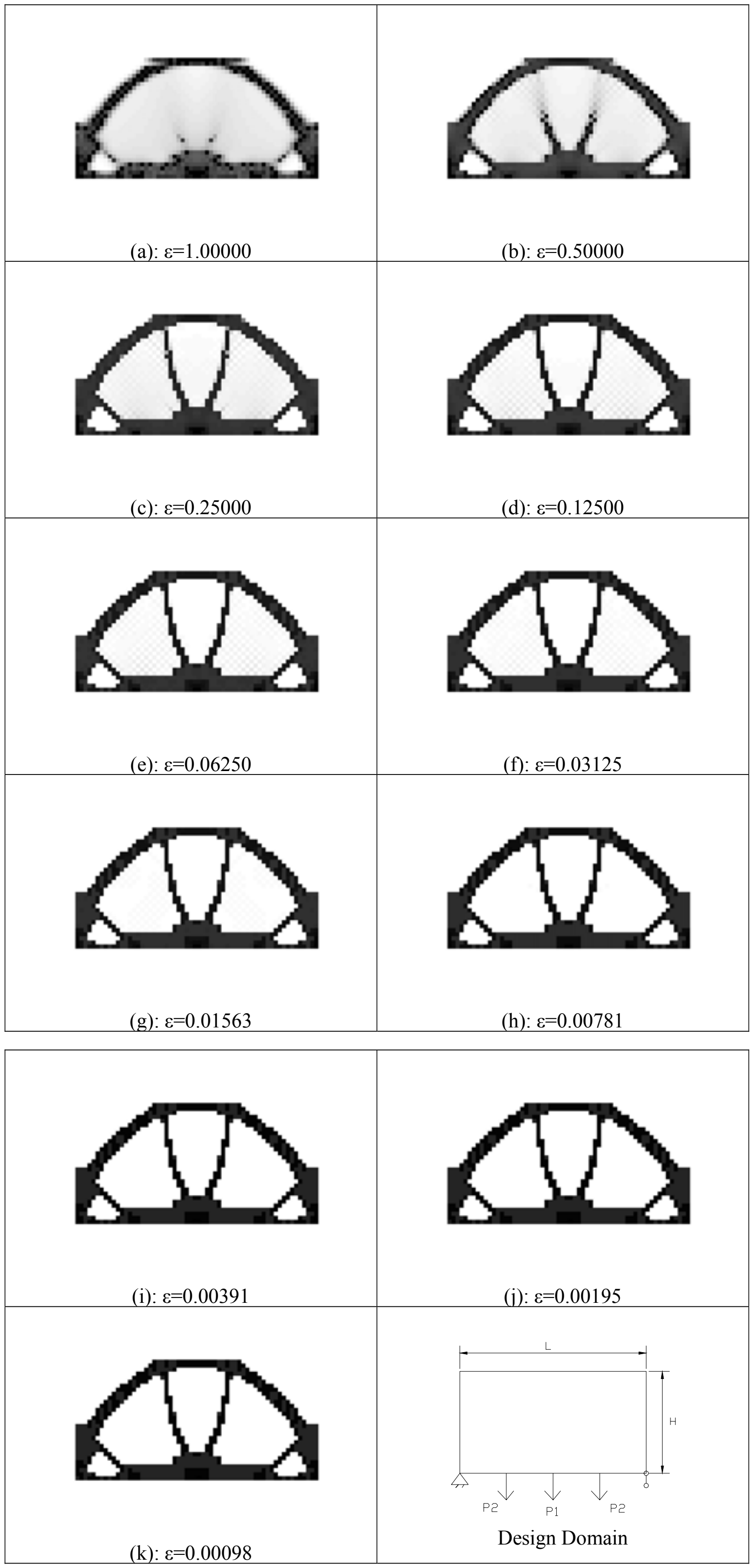

Figure 4 : A bridge type structure with fixed-simple supports. (a-k) Solutions of the Γ-convergence process, with 60×30 elements.

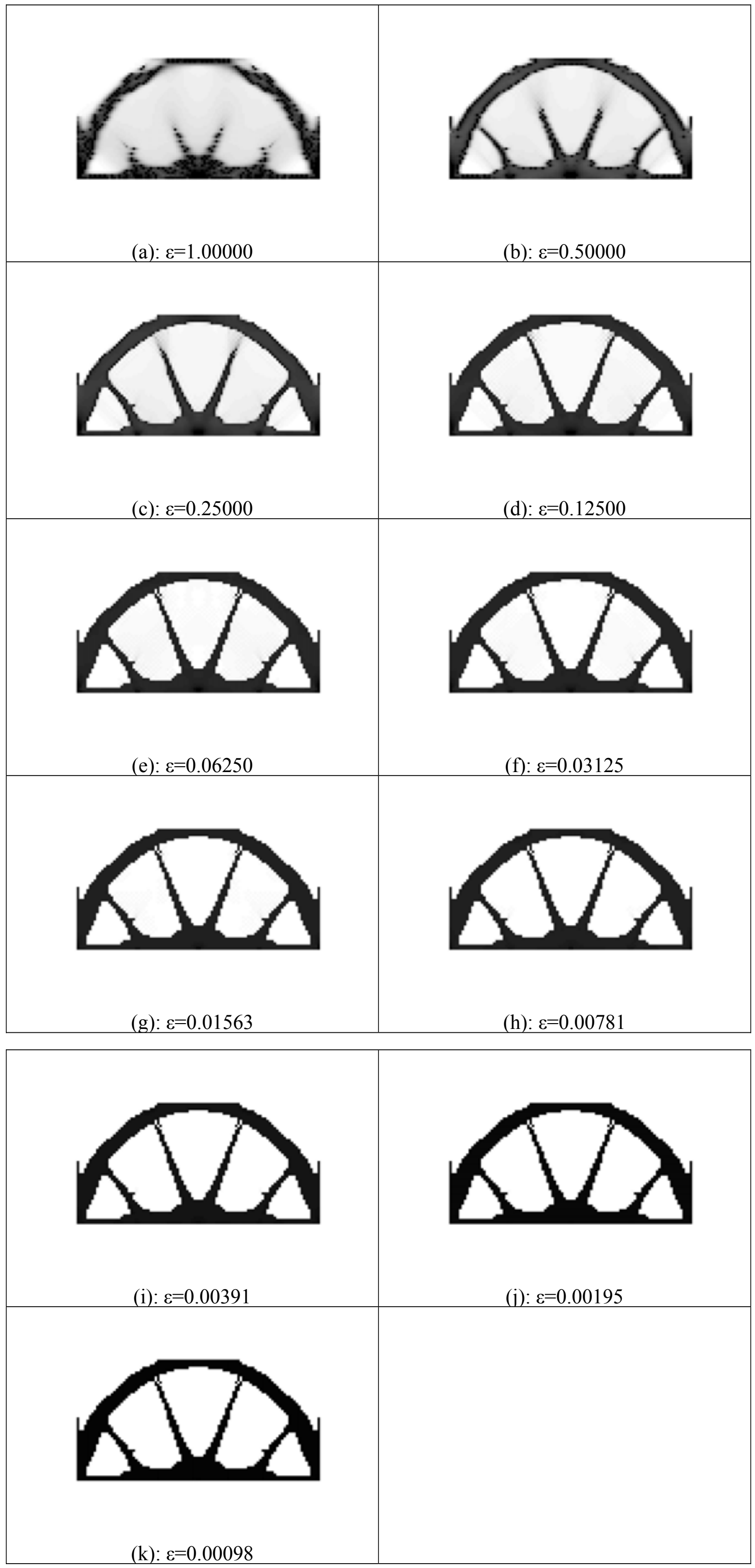

Figure 6 : The bridge structure with fixed-simple supports. (a-k) Solutions of the Γ-convergence process, with 100×50 elements.

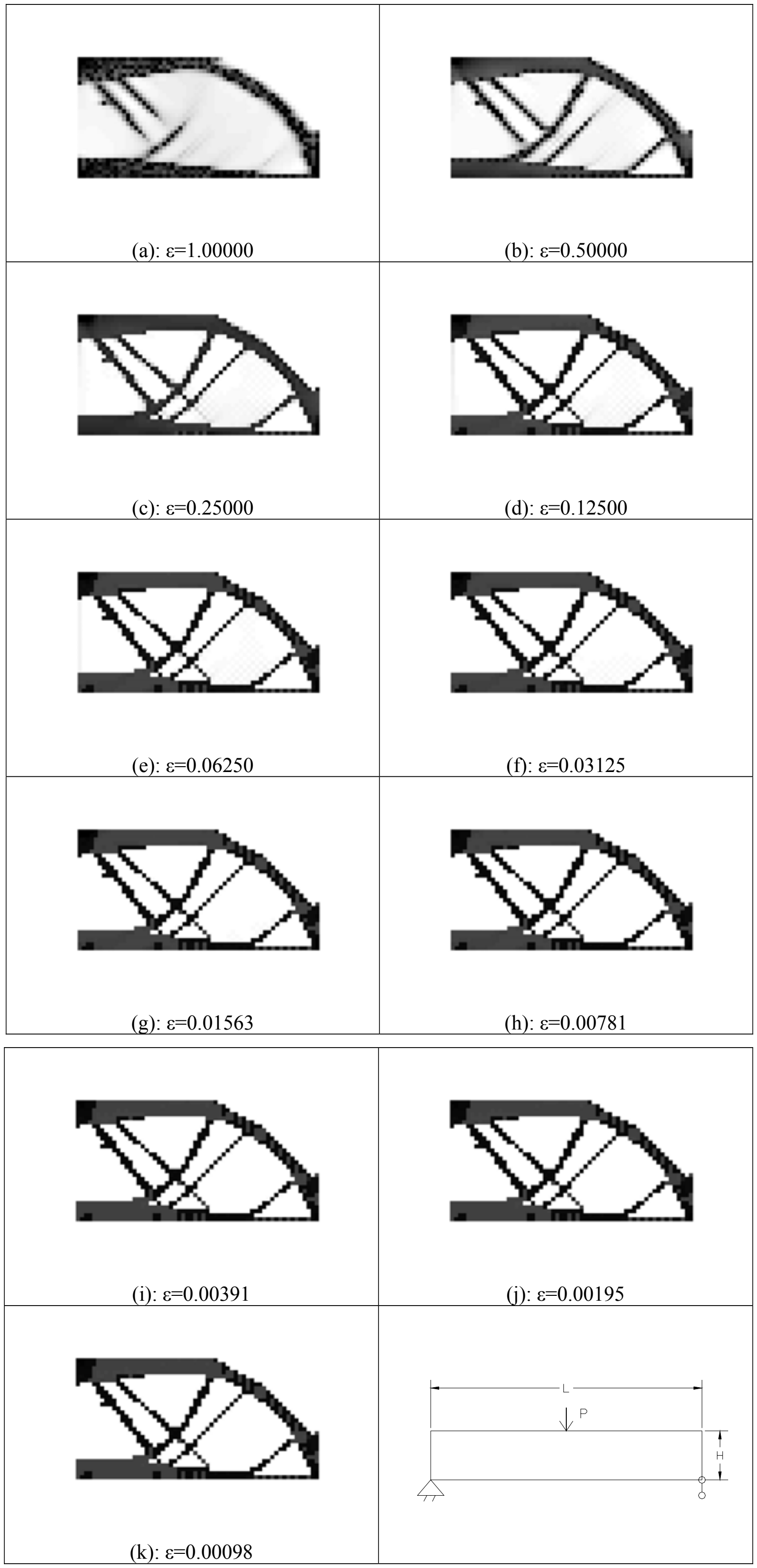

Figure 7 : The MBB structure with fixed-simple supports. (a-k) Solution sequence of the Γ-convergence process.

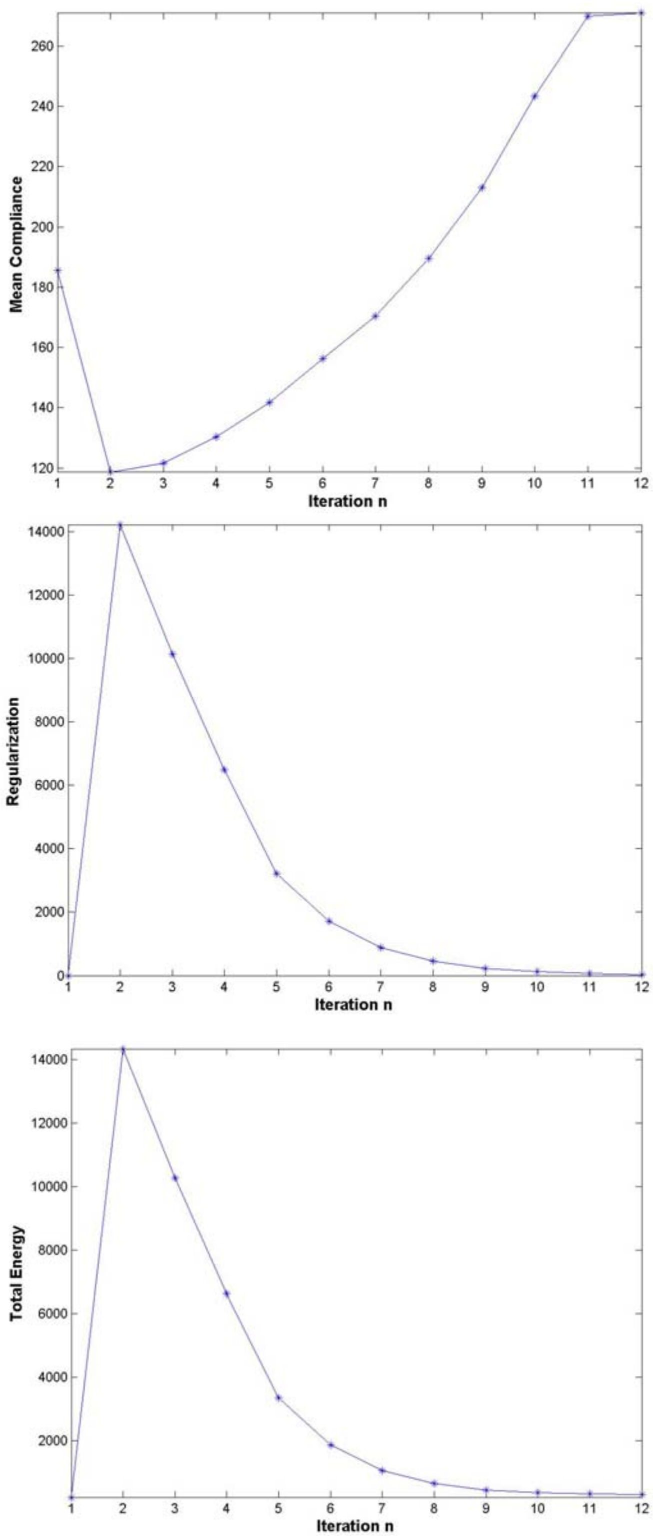

Figure 5 : The mean compliance, regularization, and total energy during the Γ-convergence process.

5.2 *MBB Beams*

This example is known as MBB beams related to a problem of designing a floor panel of a passenger airplane in Germany. The floor panel is loaded with a unit concentrated vertical force $P = 1N$ at the center of the top edge. It is has a fixed support and a simple support at its bottom corners respectively. The design domain has a length to height ratio of 12:2. The volume ratio is specified to be 0.3. We use 60×30 quadrilateral elements to model a half of the structure due to the geometric symmetry. Using the Thikonov regularization function $\varphi(s) = s^2$, we obtain the optimization sequence as shown in Fig. 7.

5.3 *Cantilever Beam*

The last example is a cantilever beam with a unit concentrated vertical force $P = 1N$ at the bottom of its free vertical edge. The design domain has a length to height ratio of 2:1. In Fig. 8 the volume ratio is specified to be 0.3, and we use 60×30 quadrilateral elements with the Thikonov regularization function.

5.4 *Effects of Different Regularization Functions*

For the three examples, other regularization functions are also employed in addition to the Tikhonov function. Fig. 9 shows the optimal designs obtained with four different regularization functions for the three examples respectively. While functions $\varphi(s) = s^2$ and $\varphi(s) = \left(1+s^2\right)^{1/2} - 1$ are convex functions, other two functions are non-convex. All of these functions produce satisfactory results.

As we discussed in Section 4.2, the auxiliary variable b in (18) in fact represents the interface (or "edges") between the solid and void, when an edge-preserving regularization function φ is used. In the phase field model, the interface is described as a diffuse interface. During the process of Γ-convergence, the interface model b tends to approach a sharp interface. This "convergence" from a diffuse interface to the sharp interface is clearly shown in Fig. 10 for the first example of the Michell structure, with $\varphi(s) = \log(1+s^2)$ for edge-preserving regularization.

5.5 *Comparison with Other Methods*

It is also interesting to compare the optimal solutions obtained for these three examples with different approaches. The SIMP method is well-known, and it is applied here with the use of the popular MATLAB code

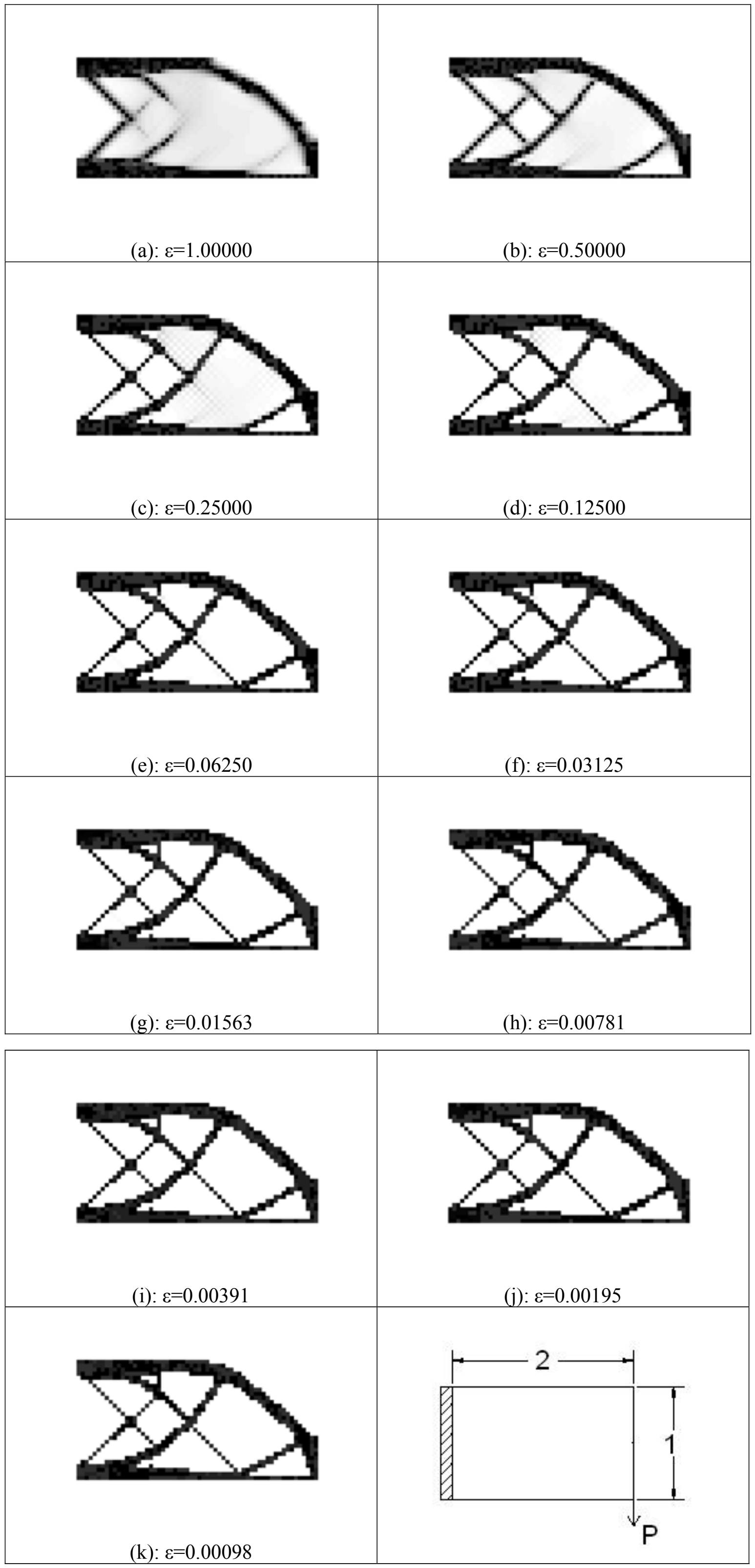

Figure 8 : The cantilever beam. (a-k) Solution sequence of the Γ-convergence process.

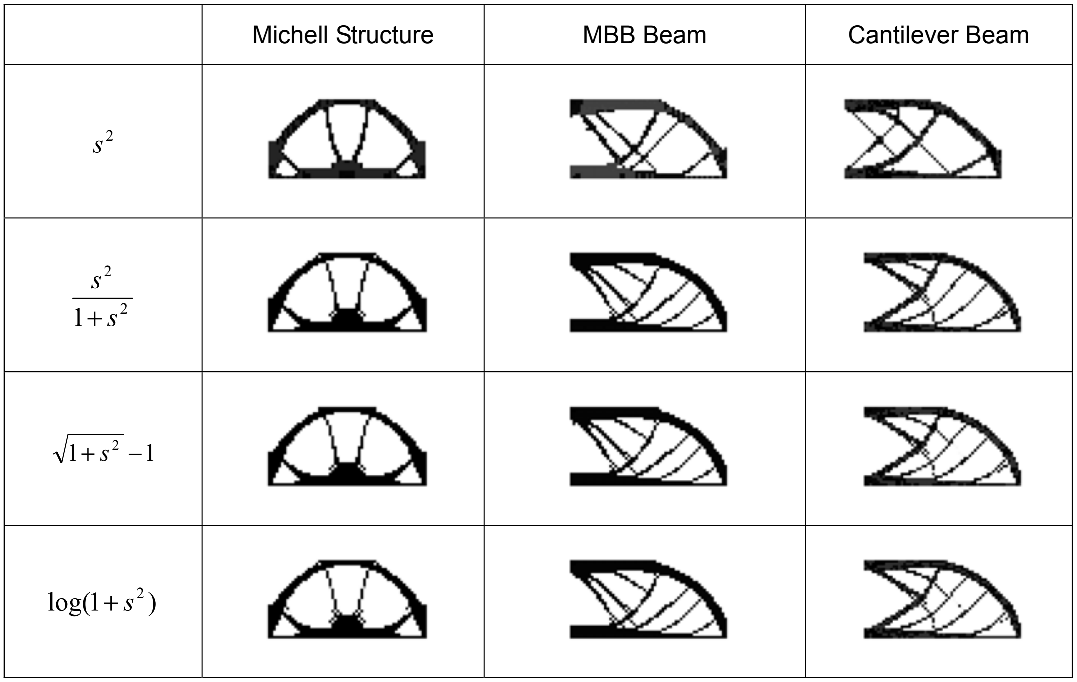

Figure 9 : Solutions of the Γ-convergence for the three examples with different φ functions

provided in (Bendsoe (2003)). We also include results of a level-set based method reported in (Wang (2003)).

As shown in Fig. 11, the three different methods, phase transition, SIMP, and level-set methods, produce very different optimal designs. It is clear that the final optimal topology of a structure depends heavily on the formulation of the problem, the geometric model, and the nature of regularization that changes the problem from being ill-posed to well-posed.

6 Conclusions and Discussions

In this paper we have presented a variational method – *phase transition* – to address the topology optimization problem. The problem is formulated as a continuous problem with the variable $0 \leq \rho(x) \leq 1$ being restricted within a fixed reference domain. However, in contrast to the widely-used material distribution approach based on homogenization, a phase-field model based on the phase-transition theory is employed. In the model, there is no distinction made between the solid, void and their interface. All regions are described in terms of the phase-field. This allows the entire design domain to be treated simultaneously, without any explicit tracking of the interface. Thus, the basic formulation of the free boundary problem of the topology optimization is replaced by a system of phase transition. We then apply the Van der Waals-Cahn-Hilliard theory to define the variational topology optimization as a dynamic process of phase transition to the system stability.

Within this variational framework, we can incorporate a regularization theory to lead to a well-posed problem formulation. We also show that the phase-field model has a close relationship with the general Mumford-Shah model of image segmentation in computer vision. These connections allow us to adapt the Γ-convergence theory for the problems of free-discontinuities and to employ a two-step, alternating numerical scheme called the half-quadratic regularization. The proposed variational method is illustrated with several 2D examples that have been extensively used in the recent literature of topology optimization, especially in the homogenization based methods.

While we have demonstrated the method only with examples of mean compliance optimization in two dimensions, this is mainly for convenience. The approach is suitable to more general optimal design problems involving multi-physics and/or multi-domains. Furthermore, the phase-field model naturally lends itself to represent

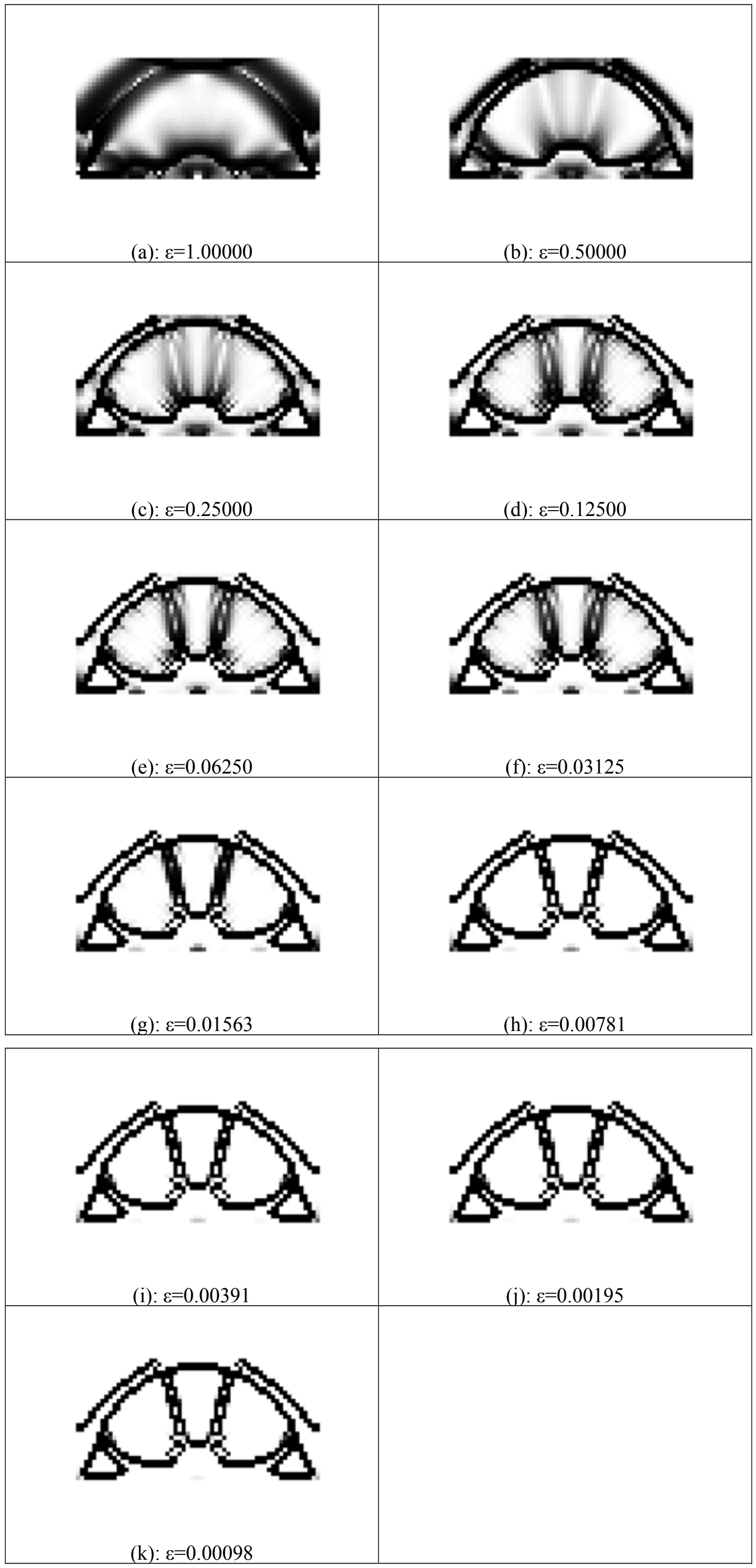

Figure 10 : The evolution of the interface model from a diffuse interface to the sharp interface for the Michell structure example

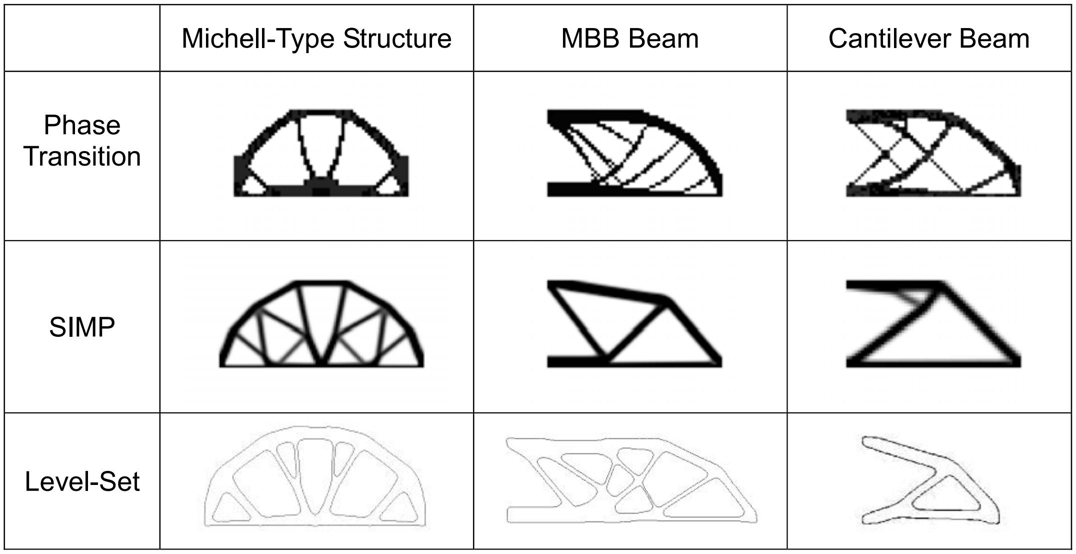

Figure 11 : Optimal designs for the three examples obtained with three different solution methods

multiple material phases other than just solid and void. In the Van der Waals-Cahn-Hilliard theory, multiple material phases are described by as many minima of the potential-well function W. Hence, there is no increase in the number of design variables, unlike the SIMP material model using a rule of mixture for multiple phases (Bendsoe (2003)). In fact, we have extended our approach to a multi-phase model for problems of optimization of heterogeneous materials and/or graded materials. The results are to be reported separately.

In view of the recent discussions on the challenges and future of the variable-topology optimization (cf. (Bendsoe (1999))), the phase-transition approach proposed here seems to be a promising alternative to the widely-used material distribution model (Bendsoe (2003)). Its further development could possibly yield optimization procedures that have more desirable features in the sense of having geometric models independent of the finite element discretization, using a relatively small number of continuous design variables, while maintaining a high flexibility in handling topological changes and mechanical analyses.

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