A PHASE-FIELD APPROACH FOR SURFACE AREA MINIMIZATION OF TRIPLY-PERIODIC SURFACES

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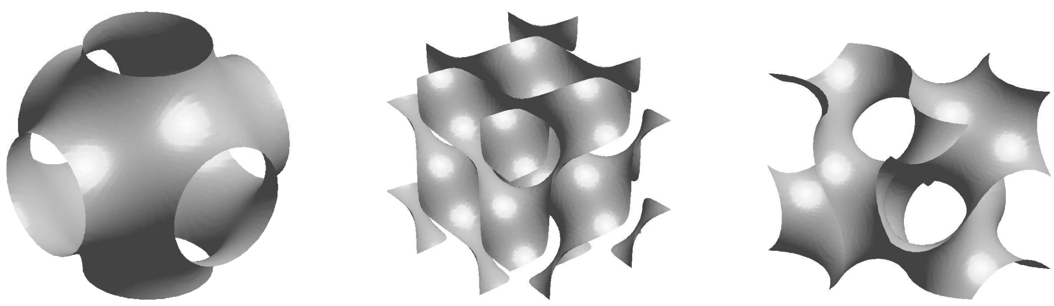
ABSTRACT

In this paper, we study triply-periodic surfaces with minimal surface area under a constraint in the volume fraction of the regions (phases) that the surface separates. Using a phase-field method formulation, we present a theoretical characterization of and a numerical algorithm for computing these surfaces. We use our theoretical and computational formulation to study the optimality of the Schwartz primitive (P), Schwartz diamond (D), and Schoen gyroid (G) surfaces when the volume fractions of the two phases are equal and explore the properties of optimal structures when the volume fractions of the two phases are not equal. Due to the computational cost of the fully three-dimensional shape optimization problem, we implement our numerical simulations using an unconditionally stable scheme and an adaptive time step scheme.



(a) (b) (c)

Figure 1. Unit cells for three different minimal surfaces: (a) Schwartz P surface, (b) Schwartz D surface, and (c) Schoen G surface.

Triply-periodic minimal surfaces [1–3] offer great attractions to physical scientists, biologists, and mathematicians. Minimal surfaces are defined as surfaces with zero mean curvature. A remarkable class of minimal surfaces are those that are triply-periodic (i.e., periodic in three directions). The Schwartz primitive (P), the Schwartz diamond (D), and the Schoen gyroid (G) minimal surfaces partition space into two disjoint but congruent regions, i.e., the volume fraction of each phase is 1/2 (see Figure 1).

In [4], using the level set method, Jung, Chu, and Torquato explored triply-periodic surfaces of nonzero mean curvature from a slightly different, but complementary, perspective. They examined the Schwartz P, Schwartz D, and Schoen G surfaces with different values for the volume fraction. The total surface area $\mathscr{A}$ is computed using

$$\mathscr{A}(\phi) = \int_{\Omega} \delta(\phi)|\nabla\phi| dV$$

and the mean curvature H is obtained from

$$\lambda = -\frac{\int_{\Omega}(\nabla \cdot \mathbf{n})\delta(\phi)|\nabla\phi| dV}{\int_{\Omega}\delta(\phi)|\nabla\phi| dV}$$

using the relation $H = 0.5\lambda$, where Ω is the entire unit cell, $\mathbf{n}$ is an outward pointing normal vector, ϕ is an embedding function, and $\delta(\phi)$ is the Dirac delta function. In their work, determined the relationship between the volume fraction, mean curvature, and surface area for the Schwartz P, Schwartz D, and Schoen G surfaces (see Figures 2-4 and Table 1).

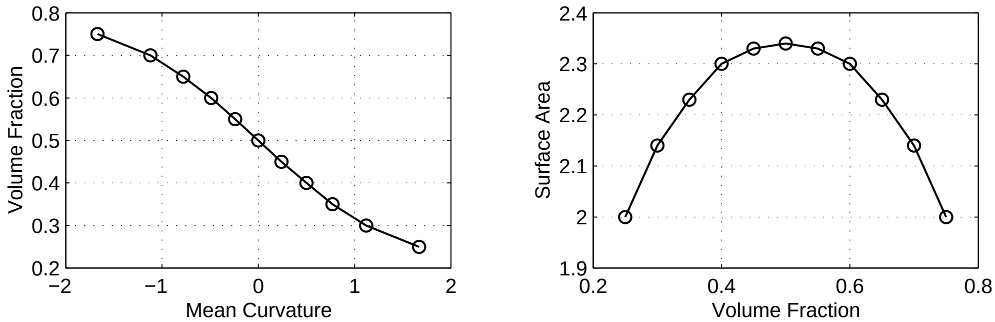


Figure 2. Relationships between the volume fraction, mean curvature, and total surface area for optimal surfaces of the Schwartz P family: volume fraction versus mean curvature (left) and total area per unit cell versus volume fraction (right).

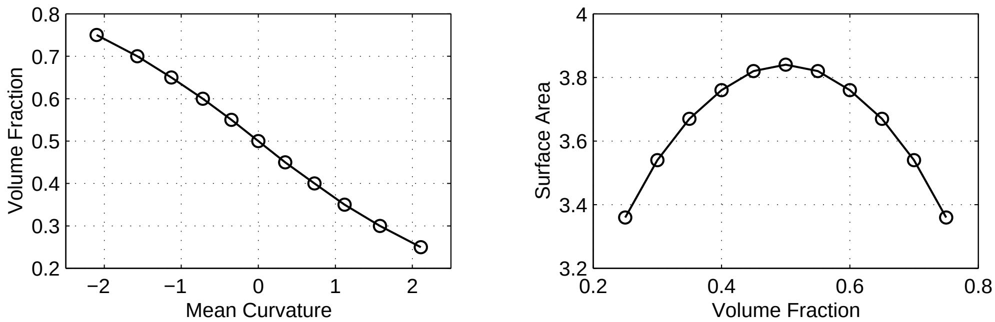


Figure 3. Relationships between the volume fraction, mean curvature, and total surface area for optimal surfaces of the Schwartz D family: volume fraction versus mean curvature (left) and total area per unit cell versus volume fraction (right).

In our numerical simulations, we use a phase-field method. We start with the free energy functional written in terms of the local volume fraction difference ϕ as

$$F[\phi] = \int_{\Omega} \left[W(\phi) + \frac{\epsilon^2}{2}|\nabla\phi|^2 \right] d\mathbf{x},$$

where $W(\phi) = 1/4(\phi^2 - 1)^2$ is free energy.

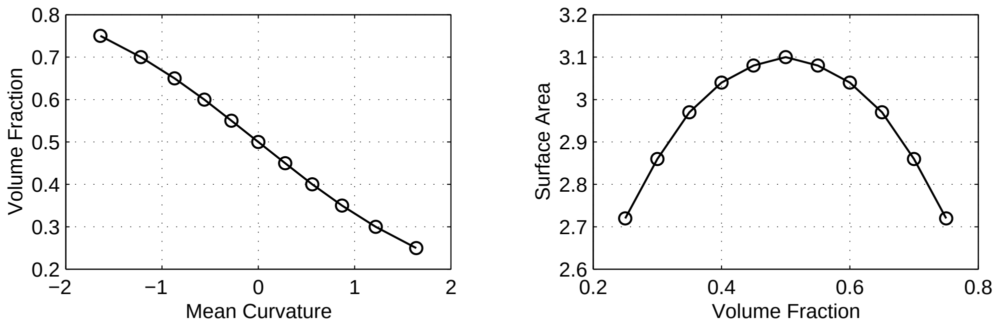


Figure 4. Relationships between the volume fraction, mean curvature, and total surface area for optimal surfaces of the Schoen G family: volume fraction versus mean curvature (left) and total area per unit cell versus volume fraction (right).

Table 1 The mean curvature and total surface area of the Schwartz P, Schwartz D, and Schoen G surfaces for different values of the volume fraction

Volume fraction, f_0	H(P)	H(D)	H(G)	$\mathscr{A}$(P)	$\mathscr{A}$(D)	$\mathscr{A}$(G)
0.25	1.67	2.11	1.64	2.00	3.36	2.72
0.3	1.12	1.58	1.22	2.14	3.54	2.86
0.35	0.77	1.12	0.87	2.23	3.67	2.97
0.4	0.50	0.73	0.56	2.30	3.76	3.04
0.45	0.24	0.35	0.28	2.33	3.82	3.08
0.5	0.00	0.00	0.00	2.34	3.84	3.10
0.55	-0.24	-0.35	-0.28	2.33	3.82	3.08
0.6	-0.49	-0.72	-0.56	2.30	3.76	3.04
0.65	-0.78	-1.13	-0.87	2.23	3.67	2.97
0.7	-1.12	-1.57	-1.22	2.14	3.54	2.86
0.75	-1.67	-2.10	-1.64	2.00	3.36	2.72

The coefficient ϵ is a positive constant. The time-evolution equation for ϕ is given by [5].

$$\frac{\partial \phi}{\partial t} = \Delta \frac{\delta F}{\delta \phi} = \Delta(\phi^3 - \phi - \epsilon^2 \Delta \phi),$$
$$\frac{\delta F}{\delta \phi} = \phi^3 - \phi - \epsilon^2 \Delta \phi.$$

Using an unconditionally stable scheme, the resulting time-stepping is:

$$\frac{\phi_{ijk}^{n+1} - \phi_{ijk}^{n}}{\Delta t} = \Delta_d \mu_{ijk}^{n+\frac{1}{2}},$$
$$\mu_{ijk}^{n+\frac{1}{2}} = \nu_{ijk}^{n+1} - \phi_{ijk}^{n},$$
$$\nu_{ijk}^{n+1} = (\phi_{ijk}^{n+1})^3 - \epsilon^2 \Delta_d \phi_{ijk}^{n+1}.$$

The above discrete system is solved by a nonlinear multigrid method.

We will compare our results from a phase-field method with ones from the level set method.

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REFERENCES

1. E.A. Lord, "Periodic minimal surfaces of cubic symmetry", *Curr. Sci.*, 85 (3), 2003, pp. 346-362.
2. A.L. Mackay, "Crystallographic surfaces", *Proc. R. Soc. Lond.*, A 442, 1993, pp. 47-59.
3. J. Klinowski, A.L. Mackay, H. Terrones, "Curved surfaces in chemical structure", *Phil. Trans. R. Soc. Lond.*, A 354, 1996, pp. 1975-1987.
4. Y. Jung, K.T. Chu, S. Torquato, "A variational level set approach for surface area minimization of triply-periodic surfaces", *J. Comp. Phys.*, 223, 2007, pp. 711-730.
5. D.J. Eyre, "An unconditionally stable one-step scheme for gradient systems", Unpublished article, 1998.