A free boundary problem for anisotropic surface energy

Miyuki Koiso*(Kyushu University. Joint work with Y. Jikumaru)

June 6, 2024

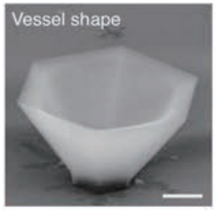
The 81st Fujihara seminar

“Mathematical Aspects for Interfaces and Free Boundaries”

*Partially supported by JSPS KAKENHI JP23K20212 and JST CREST JP MJCR1911.

1 Introduction

Here are two photos of single crystals and a picture drawn by PC.



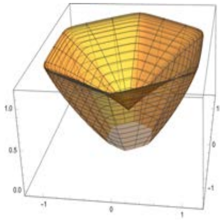


Figure 1: **Left: crystal of salt in water. Center: microcrystal on a quartz substrate. Right: equilibrium surface for an anisotropic surface energy (§5)**

Most of single crystals are convex. However, the crystal in Fig.1, center is not convex. It is grown from an S-planarchiral aromatic molecule [2.2] paracyclophane appended with four (methoxyphenyl) ethynyl arms (Oki et al., 2022, Science). They say morphology, size, and orientation of such non-convex crystals are difficult to control because they grow quickly. In this talk we study equilibrium shapes of anisotropic surface energy which may be applicable to single crystals.

The subject of this talk is generalized to hypersurfaces in $\mathbf{R}^{n+1}$. Also the methods we will discuss are essentially very general. However, in order to save time, I will mainly discuss surfaces in $\mathbf{R}^3$, explain the methods for specific examples, and some results will be given under stronger assumptions than their original theorems.

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2 Anisotropic surface energy (energy of crystals)

Let $\gamma : S^2 = \{\nu \in \mathbf{R}^3; |\nu| = 1\} \to \mathbf{R}_{>0}$ **be a** C^0 **function, (energy density),**
$M = \cup_{i=1}^k M_i$, **a closed oriented piecewise-**C^2 **surface in** R^3**,**
$\partial M_i \cap \partial M_j = M_i \cap M_j$, **if** $i \neq j$**.** M_i **is smooth with unit normal** ν**.**

The anisotropic (surface) energy $\mathcal{F}_\gamma(M)$ **of** M **is defined as follows:**

$$\mathcal{F}_\gamma(M) := \sum_{i=1}^k \int_{M_i} \gamma(\nu(p))\, dA.$$

If $\gamma \equiv 1$, $\mathcal{F}_\gamma(M)$ **is the usual area of** M**.**

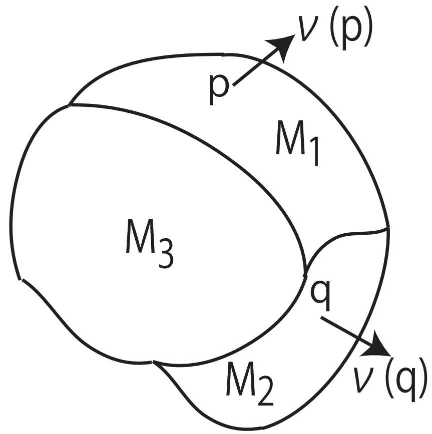

Figure 2: **A piecewise-C² surface with unit normal** ν

For any $V > 0$, among all closed surfaces enclosing the volume V, there exists a unique (up to translation) minimizer $W_\gamma(V)$ of $\mathcal{F}_\gamma = \int \gamma(\nu) dA$ (J. E. Taylor,'78). For a certain specific $V_0 > 0$, $W_\gamma(V_0)$ is called the Wulff shape for γ, which will be denoted by W_γ. All $W_\gamma(V)$ are homothetic to W_γ.

Example 2.1. (i) If $\gamma \equiv 1$, the Wulff shape W_γ is the unit sphere S^2.
(ii) If $\gamma(\nu) = \gamma(\nu_1, \nu_2, \nu_3) = |\nu_1| + |\nu_2| + |\nu_3|$, ($\nu \in S^2$), W_γ is the cube $\{x = (x_1, x_2, x_3) \in \mathbf{R}^3 \mid \max\{|x_1|, |x_2|, |x_3|\} = 1\}$.

(iii) If $r > 0$, $h > 0$, and $\gamma(\nu) = r\sqrt{\nu_1^2 + \nu_2^2} + h|\nu_3|$, W_γ is the cylinder with radius r and height $2h$.

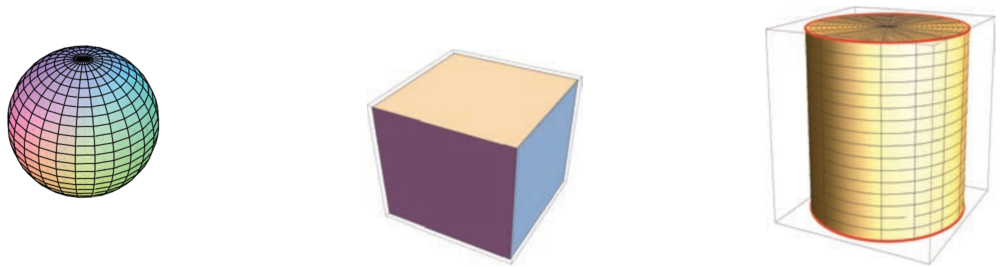

Figure 3: **Wulff shapes for γ's in Example 2.1: sphere, cube, cylinder.**

3 Cahn-Hoffman map and anisotropic mean curvature

The homogeneous extension of $\gamma : S^2 \to \mathbf{R}_{>0}$ is defined as follows.

$$\overline{\gamma} : \mathbf{R}^3 \to \mathbf{R}_{\geq 0}, \qquad \overline{\gamma}(rX) := r\gamma(X), \ \forall X \in S^2, \ \forall r \geq 0.$$

We say that γ is convex if and only if $\overline{\gamma}$ is a convex function.

Assume γ is of C^1. The map $\xi_\gamma : S^2 \to \mathbf{R}^3$ defined by $\xi_\gamma(\nu) := D\overline{\gamma}|_\nu$, ($\overline{D}$ is the gradient in $\mathbf{R}^3$) is called the Cahn-Hoffman map for γ.

In general, $W_\gamma \subset \xi_\gamma(S^2) =: \tilde{W}_\gamma$.

γ is a convex integrand. $\iff W_\gamma = \xi_\gamma(S^2)$.

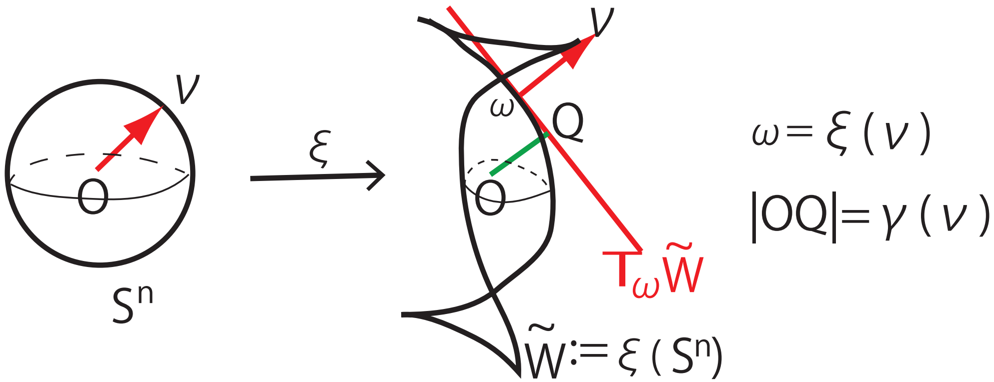

Figure 4: **The Cahn-Hoffman map $\xi_\gamma : S^2 \to \mathbf{R}^3$**

Definition 3.1 (anisotropic mean curvature). $\Lambda := (1/2)(-\mathrm{div}_M D\gamma + 2H\gamma)$ is called the anisotropic mean curvature of M, where H is the mean curvature of M.

If γ is convex, "$\Lambda \equiv$ constant" is a 2nd order quasi-linear elliptic PDE.
By using the first variation formulas of the the anisotropic energy and the volume (see the next slide), we see:

Proposition 3.1. [Euler-Lagrange eqns] **Assume $\gamma \in C^2(S^2)$. A piecewise-C^2 surface $M = \cup M_i \subset \mathbf{R}^3$ is a critical point of the anisotropic energy $\mathcal{F}_\gamma(M) = \int_M \gamma(\nu)\, dA$ for volume-preserving variations if and only if**

(i) $\Lambda \equiv$ **constant on M, and**

(ii) $(G|_{M_i} - G|_{M_j})(\zeta) \in T_\zeta(\partial M_i \cap \partial M_j)$ **at** $\forall \zeta \in \partial M_i \cap \partial M_j$. **($G = \xi_\gamma \circ \nu$.)**

If M satisfies the above (i) and (ii), we call M a CAMC surface.
The image of the Cahn-Hoffman map has $\Lambda = -1$ at regular points.

First variation formulas:

Lemma 3.1. **Assume that $M \subset \mathrm{R}^3$ is a smooth surface with unit normal ν. Let $M_\epsilon = M + \epsilon(\delta M) + \mathcal{O}(\epsilon^2)$ be a smooth variation of M. Then the first variation of the anisotropic energy $\mathcal{F}_\gamma$ is given as follows.**

$$\delta \mathcal{F}_\gamma \quad := \quad \frac{d\mathcal{F}_\gamma(M_\epsilon)}{d\epsilon}\Big|_{\epsilon=0} = -\int_M 2\Lambda\langle \delta M, \nu\rangle \, dA - \oint_{\partial M} \langle \delta M, R(p(\xi_\gamma \circ \nu))\rangle \, d\tilde{s},$$

where dA is the area element of M, N is the outward-pointing unit conormal along ∂M, $d\tilde{s}$ is the line element of ∂M, R is the $\pi/2$-rotation on the (N, ν)-plane, and p is the projection from R^3 to the (N, ν)-plane.

Moreover it is known that the first variation formula of the volume enclosed by M is given as follows.

$$\delta V = \int_M \psi \, dA, \qquad \psi := \langle \delta M, \nu \rangle. \tag{1}$$

4 Uniqueness of closed CAMC hypersurfaces

Is a closed CAMC hypersurface in $\mathbf{R}^{n+1}$ only the Wulff shape?

	regularity	$n=2$, genus 0	$\forall n$, stable	$\forall n$, embedded
$\gamma \equiv 1$ ($W = S^n$)	smooth	◯ Hopf '51	◯ Barbosa-do Carmo'84	◯ Alexandrov '62
$\gamma, W_\gamma \in C^\infty$, $D^2\gamma + \gamma 1 > 0$	smooth	◯'10 K-Palmer 2012 Ando	◯ 1998 Palmer	◯ He-Li-Ma-Ge, 2009
$\gamma \in C^2$ γ:convex	piecewise C^2, non-flat	?	(2012 Palmer) ◯ 2018 Koiso	?
$\gamma \in C^0$ Lip γ:convex (e.g. crystal)	can have flat faces (cf.discrete surface)	?	? $n=1$ ◯'05 Morgan	?
$\gamma \in C^\infty$ non-convex	piecewise smooth, non-flat	× Jikumaru-K 2018	?	× Jikumaru-K 2018

5 A (free) boundary problem

Let M be CAMC. For volume-preserving variation with variation vector field $\delta M = \eta + \psi\nu$, the second variation of the energy is given by

$$\delta^2 \mathcal{F}_\gamma = -\int_M \psi L[\psi]\, d\Sigma + \oint_{\partial M} \psi \langle A\nabla\psi, n\rangle\, d\tilde{s}, \tag{2}$$

where L is the self-adjoint Jacobi operator

$$L[\psi] := \mathrm{div}(A\nabla\psi) + \langle A d\nu, d\nu\rangle\psi,$$

$A := D^2\gamma + \gamma 1$, and n is the outward-pointing unit conormal along ∂M. Note that $L[\nu_i] = 0$ ($\nu = (\nu_1, \nu_2, \nu_3)$). In order to check the stability of CAMC surfaces, it is useful to study the following eigenvalue problem.

$$L[\psi] = -\lambda\psi \text{ on } M, \quad \nabla\psi|_{\partial M} = 0. \tag{3}$$

Now, fix a positive energy density function $\gamma : S^2 \to \mathbf{R}_{>0}$ and a plane Π. Consider the following free boundary problem:

(FB) Study equilibrium surfaces of the anisotropic energy $\mathcal{F}_\gamma$ for surfaces with free boundary on the plane Π enclosing a given volume.

M is a solution of (FB) iff M is CAMC and orthogonal to Π.

Definition 5.1. A solution $M = \cup_{i=1}^{k} M_i$ of (FB) is said to be stable if the second variation of $\mathcal{F}_\gamma$ for any volume-preserving variation satisfying the boundary condition is non-negative.

It is easy to show:

Proposition 5.1. Let M be a solution of (FB). Assume that M is a graph of a function defined on a domain in Π. If the equation "$\Lambda =$constant" is elliptic, then M is stable.

Now, we give an example. Set $r(t) := \left[\cos^8\left(\frac{3t}{2}\right) + \sin^8\left(\frac{3t}{2}\right)\right]^{-\frac{1}{20}}$**.**
Consider a surface $S : (x, y, z)$ **(**$-\pi/2 \le \theta \le \pi/2$**,** $0 \le t < 2\pi$**) defined by**

$$x = \left[6\cos^4\theta - 5(\cos^6\theta + \sin^6\theta)\right](\cos\theta)r(t)\cos t, \tag{4}$$

$$y = \left[6\cos^4\theta - 5(\cos^6\theta + \sin^6\theta)\right](\cos\theta)r(t)\sin t, \tag{5}$$

$$z = \left[6\sin^4\theta - 5(\cos^6\theta + \sin^6\theta)\right]\sin\theta. \tag{6}$$

Define $\gamma : S^2 \to \mathbf{R}$ **so that the image of the Cahn-Hoffman map** ξ_γ **is** S**.**

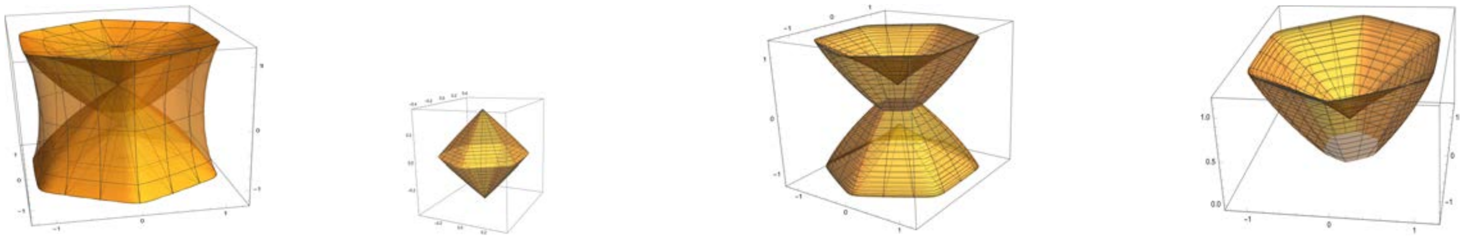

Figure 5: S, W_γ, **a closed CAMC surface and its upper half.**

The right end surface $M = M_1 \cup M_2$ **in Fig.5 is stable for variations which do not break the smoothness of each** M_i **for fixed boundary.** **How about the stability when the smoothness is changed is open.**

References

[1] **Y. Jikumaru and M. Koiso. Non-uniqueness of closed embedded non-smooth hypersurfaces with constant anisotropic mean curvature, preprint. arXiv:1903.03958 [math.DG]**

[2] **M. Koiso, Uniqueness of stable closed non-smooth hypersurfaces with constant anisotropic mean curvature, preprint. arXiv:1903.03951 [math.DG]**

[3] **M. Koiso, Uniqueness of closed equilibrium hypersurfaces for anisotropic surface energy and application to a capillary problem, Mathematical and Computational Applications, (2019), 24(4), 88; https://doi.org/10.3390/mca24040088**