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IS THERE GRAVITY-INDUCED FACETTING OF CRYSTALS?

by Jean E. TAYLOR (Rutgers University)

1. INTRODUCTION.

The question of the shape of a drop of fluid sitting on a table in a gravitational field has been studied analytically for 180 years, from Laplace [4] to Finn [3]. But solids have surface energy as well, so this question makes equally good sense in that case. For a single crystal of a solid, the surface energy per unit area (for a fixed orientation of the crystal) usually depends continuously on the normal direction, and the gravity-free shape is normally not a sphere.

In this paper, the following two results are proved in the case that the gravity-free shape is polyhedral and has an edge pointing up:

1) In the absence of special symmetry, no gravity-induced facet can occur on top of a convex crystal (Theorem 1), and

2) In some special symmetric cases, a gravity-induced facet must occur for sufficiently large values of the gravitational constant, provided the body is convex (Theorem 2).

More precisely, the surface tension of the crystal-medium interface is a continuous function

$$F : S^2 \to R^+ = R \cap \{r\colon r>0\}$$

and the surface energy $E_S(V)$ of a region V of finite perimeter contained in the half space $H = \{x \in R^3\colon x_3 \geq 0\}$ is

$$E_S(V) = \int_{x\in \partial V \cap \{x:\ x_3>0\}} F(\nu(x))\, d\mathcal{H}^2 x + \sigma\, \mathcal{H}^2(\partial V \cap \partial H);$$

here $\nu(x)$ is the exterior normal of the reduced boundary of V (see [2, 4.5.6]; it is hereafter denoted ∂V) for all x in ∂V and σ is the difference between the surface tension of the crystal-table interface and table-medium interface. As usual, the gravitational energy $E_G(V)$ is

$$g\int_{x\varepsilon V} x_3 \, d\mathcal{L}^3 x,$$

where g represents the gravitational constant times the difference in density between the material of V and the surrounding medium.

Thus the question of the equilibrium shape of a crystal of volume v sitting on a table in a gravitational field, with given F, σ, and g, is the question of the shape of any minimizer of $E(V) = E_S(V) + E_G(V)$ in the class of sets of finite perimeter of having volume v and being contained in H.

Since surface energies vary with direction, the notions of wetting and contact angles and their relationship to σ are much more elaborate than in the isotropic case and it seems best to leave the problem in its energy formulation.

For $g = 0$, the problem has been completely solved and the result (called W throughout this paper) is unique and convex; see section 2 below. For $g > 0$, it is not even known if a solution must be convex, or indeed if <u>any</u> solution is convex. (The case of a two-dimensional crystal is sufficiently special that it also is essentially completely solved; see [1]. In particular, those solutions are also unique and must be convex.)

In [1] it was shown that if W was polyhedral and had a corner [resp., edge] pointing up, and if solutions to the $g > 0$ case were convex [resp., convex and polyhedral], then gravity-induced facetting on top resulted if the gravitational constant was large enough relative to the volume enclosed.

In this paper, it is shown that the hypothesis of V being polyhedral was crucial: examples are given of surface tension functions for which there is never a facet on top, as well as ones for which there is a facet on top for large enough g.

2. THE ZERO-GRAVITY SOLUTION.

Given $F : S^2 \to R^+$, the region of given volume with least surface energy in the interior of H exists and is unique up to translation (see [5] for proofs and further references); its shape is given by the Wulff construction

$$W = \{x \in R^3: x \cdot n \leq F(n) \quad \text{for every} \quad n \in S^2\}.$$

W can then be scaled by a homothety to achieve the desired volume and translated to lie inside H. W itself is called the crystal of F. The solution to the related free-boundary problem, where the region is allowed to contact ∂H, can also be found by the Wulff construction, in the sense that the solution is

$$W' = \tau(W \cap \{x: -x_3 \leq \sigma\}),$$

where $\tau: R^3 \to R^3$ is the translation $\tau(x_1,x_2,x_3) = (x_1,x_2,x_3+\sigma)$ (see [6]). If $-\sigma > \max\{x_3: x \in W\}$, then W' has zero volume; this corresponds to the case of complete wetting, where the region degenerates to a thin film completely covering ∂H. If $-\sigma < \min\{x_3: x \in W\}$, there is complete drying, and there is an infinitesimal film of the medium between the material of V and the table; the shape of V is identical, however, to that when $-\sigma = \min\{x_3: x \in W\}$.

3. ASSUMPTIONS AND NOTATIONS.

Throughout this paper, we fix an F such that W is polyhedral (such integrands are called crystalline). We assume further that only 3 facets meet at each corner of W. We fix a $g > 0$ and a σ such that

$$\min\{x_3: x \in W\} \leq -\sigma < \max\{x_3: x \in W\}.$$

It is convenient to assume further that F is a convex function, since then E(V) is a lowersemicontinuous function. This can be done without loss of generality in the following sense, as shown in [5].

Let G be the (unique) convex integrand having W as its Wulff shape. Then $G(n) = F(n)$ for each n which is a normal to W, and G is determined by its values on the set of normals to W. Any set of finite perimeter V has a corresponding varifold V' with V as underlying set such that the surface energy of V, using G, is the same as that of V', using F. V' can be thought of as having "infinitesimal corrugations" wherever it has tangent planes with normals that are not normals to W. We therefore do assume that F is convex, and we simply observe at the end that if any solution V has a normal n which is not a normal to W, V can be replaced by the corresponding varifold V' to obtain a solution to the original problem with nonconvex F.

Finally, we define F' by $F'(n) = F(n)$ if n is not $(0,0,-1)$, and $F'((0,0,-1)) = \sigma$.

We denote by V (or, to emphasize the dependence on g, occasionally by V_g) any minimizer of the total energy $E_G + E_S$.

Normal directions to W are called crystalline directions; all other directions are called noncrystalline directions.

4. THE CRYSTAL GRAPH.

The dual graph of W' (called the crystal graph) can be defined since W' is a polyhedron (it is the subdivision of the unit sphere induced by the Gauss map on W'): there is a vertex in S^2 for every facet of W', this vertex being the normal to that facet, and there is an edge between two vertices if and only if the corresponding facets intersect along a line segment, that edge being the shorter geodesic between the vertices. Each face of the dual graph then corresponds to a corner of W'.

5. SUMMARY OF PREVIOUS RESULTS FROM [1] (assuming W is polyhedral).

1) The normals to V lie in the closure of the union of the edges of the crystal graph.

2) If V_g is convex and if W has an edge on top, then for large enough g V_g either has a facet or is curved on top; if V_g is polyhedral near its top, then V_g has a facet on top for large enough g.

3) The quantity

$$\lambda = (2\ E_S + 4\ E_G)/3v$$

serves as a "Lagrange multiplier" in this problem. A typical initial deformation will change the volume by a small amount Δv, change E_S by an amount ΔE_S, and change E_G by an amount ΔE_G. The new region is then rescaled to the original volume by the scale factor $s = (v/(v + \Delta v))^{1/3} \approx 1 - \Delta v/3v$; the surface energy scales by s^2 and the gravitational energy by s^4. Thus the net change in energy due to the combined deformations is

$$\Delta E = \Delta v(\Delta E_G/\Delta v + \Delta E_S/\Delta v - \lambda) + O((\Delta v^2).$$

Letting h be the maximum height of V, we note that $\lambda - gh \geq 0$ since one such deformation involves pushing down on the top of V $(\Delta v < 0)$, giving $\Delta E_G/\Delta v \approx gh$, $\Delta E_S/\Delta v \geq 0$, and thus

$$0 \leq \underline{\lim}\ \Delta E/\Delta v \leq -gh + \lambda.$$

6. NEW RESULTS.

Lemma. a) *If* $x \in \partial V$, N *is a convex neighborhood of* x, *and* $V \cap N$ *is convex, then* ∂V *has a unique tangent cone at* x, *and this tangent cone is a cone;*

b) *Tangent cones to* ∂V *minimize* E_S*;*

c) *Under the hypotheses of a), the normals to the tangent cone lie on the boundary of a single face of the crystal graph.*

Proof. Parts a) and b) are well-known and easily checked (the tangent cone is the translation to the origin of the boundary of the intersection of all supporting half-spaces of V N at x, and tangent cones minimize E_S alone because surface and volume integrals scale differently under homotheties). If part c) were not true, there would be a unit vector n_0 inside the convex hull on the sphere of the normals to the cone such that n_0 is a vertex or on an edge of the crystal graph. One could then deform the cone by flattening it near its vertex, producing a facet with normal n_0; this deformation decreases surface energy, by calculations analagous to those in [5].

Proposition.

Hypotheses:

1) V *minimizes the total energy*

2) $x \in \partial V$, ∂V *has normal* n *at* x, *and* n *is inside the edge of the crystal graph corresponding to an edge* T *of* W

3) $V \cap N$ *is convex, where* N *is a convex neighborhood of* $\tau \cap V$ *and* τ *is the line through* x *parallel to* T.

Conclusions:

1) $\partial V \cap \tau$ *is a line segment (hereafter called a ruling) of positive length*

2) $\ell(\lambda - gh) = L$, *where* λ *is the "Lagrange multiplier" and*

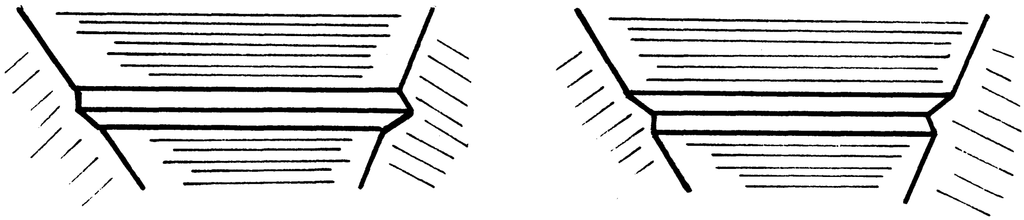
ℓ *is the length of the ruling through* x

h *is the height of the center of gravity of this ruling*

L *is the length of* T *in* W.

Proof. Let V, n, T, ℓ, h, and L be as in the hypotheses. Let m be a unit vector orienting T. Using the convexity of $V \cap N$ and summary fact 1, we see that $V \cap \tau$ is a line segment of positive length, and a general position argument allows us to assume that V has tangent cones consisting of two half planes at each end of τ. Let n_e denote the normal other than n to that tangent cone at the positive end of T and let n_b denote the other normal at the negative end.

We consider the deformations illustrated below. They push in or out a



furrow or ridge at x of depth d parallel to T, with the normals to the long sides being the normals n_1 and n_2 of the facets of W containing T and, in the case of a ridge, with roughly triangular patches at the ends with normals n_e and n_b as appropriate (in the case of a furrow, the deformation cuts away such triangular pieces at the ends). If we denote the cross-sectional area perpendicular to T of the furrow or ridge by ad^2, then the surface energy of the triangular regions added or cut off at the ends is

$$ad^2\,(F(n_e)/m.n_e + F(n_b)/|m.n_b|) + O(d^3)$$

and the volume change is $ad^2 + O(d^3)$. One can compute the remaining terms in the change of surface energy directly; alternatively and more instructively, one can let w_0 be the coordinate vector of the corner of W at the n_b end of T, so that $w_0 + Lm$ is the coordinate vector of the n_e end. The surface energy of W and of V does not depend on the center of W, by the divergence theorem; therefore the computation of the change in surface energy cannot depend on the value of w_0 and we may compute this change with w_0 equal to $(0,0,0)$. Now $F(n_b) = F(n_1) = F(n_2) = 0$, and the change in surface energy depends only on $F(n_e) = L\, m.n_e$ (and the geometry of the piece with normal n_e); hence it is

$$ad^2L + O(d^3).$$

Therefore after applying a homothety to restore the original volume, one obtains

$$0 = \Delta E = \Delta v(-\lambda + gh + L/\ell) + O(d^3),$$

and hence

$$\ell(\lambda - gh) = L.$$

Corollary 1. *Any facet with a noncrystalline direction* n *is a parallelogram with constant* ℓ *and* h *and hence has horizontal ends and (unless* $n = (0,0,1)$*) nonhorizontal rulings.*

Proof. A facet on a convex body must itself be convex; thus $\ell(\lambda - gh) = L$ (a constant) implies that ℓ and h are constant.

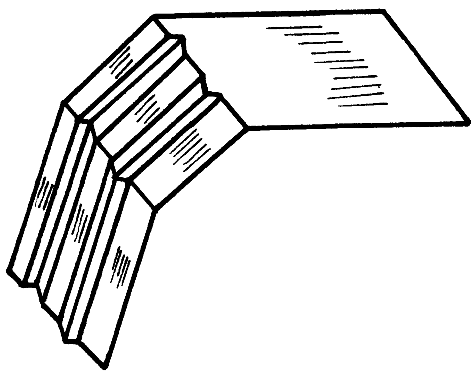
Corollary 2. *Any continuous family of normal directions to* V *such that one set of the ends of its rulings are in a horizontal plane has the other set of ends in another horizontal plane.*

Proof. Under the above hypotheses, ℓ and h are affinely related ($h = h_0 + c\ell/2$, where h_0 is the height of the horizontal plane and the absolute value of c is the square root of $1 + (n.n_e)^2$) and therefore each must be constant.

Theorem 1. *Suppose that* W *is such that each great circle on the unit sphere through* $(0,0,1)$ *contains at most one normal to* W *in addition to* $(0,0,-1)$*, and that* $(0,0,1)$ *is in an edge of the crystal graph. Then there is no facet on top of any convex* V_g *which minimizes the total energy, for any value of the gravitational constant.*

Proof. Suppose that W and V are as in the hypotheses, but that V does have a facet with normal $(0,0,1)$. By Corollary 1, this facet must be a parallelogram, and the normals to the tangent cones at the ends of the facet both must lie on a great circle through $(0,0,1)$. By the hypotheses on W, there are no crystalline directions in at least one of the two half circles from $(0,0,1)$ to $(0,0,-1)$ in this great circle; we restrict ourselves to an end of the top facet whose tangent cone normals are in such a half circle. Since all normals to V are in the closure of the edges of the crystal graph, there must be a facet with a noncrystalline direction at this end of the top facet; by corollary 1, it too is a parallelogram. Similarly, it too has a parallelogram coming off its lower edge, and so forth, down to a facet with its lower edge in the plane $x_3 = 0$. (The finiteness of the number of edges in the crystal graph ensures that there are a finite number of parallelograms in this string.)

In this situation there is a deformation with net energy change precisely zero which changes the lengths of some of the rulings in the top facet, as indicated in the figure. Shallow similar triangles of equal area are pushed out



and pushed into the top facet at the end under discussion. Each ruling in its adjacent facet which ended on one edge of a triangle is moved out or in horizontally, extending or shrinking a ruling of the top facet, until it reaches one of the other edges of the triangle. This creates two triangles of the same area in the horizontal plane containing the lower edge of this facet. The next facet down then has its ruling translated as above, and so forth, until the plane $x_3 = 0$ is reached. If the triangles are shallow enough that all normals of the deformed surface stay within their respective edges of the crystal graph, then the total surface energy change is precisely zero, since it is zero with respect to each facet (including the one with normal $(0,0,-1)$). The change in volume is 0, since equal areas are added and subtracted at each height; similarly, the change in gravitational energy is precisely zero.

Finally, the existence of this deformation provides a contradiction, since the deformed surface, having the same energy, must also be a minimum for the total energy, and yet the rulings on the top facet are not of equal length, contradicting corollary 1.

Theorem 2. *Suppose that the crystal graph has five vertices, one being* (0,0,-1) *and the other four having edges to* (0,0,-1), *with two of these vertices being joined by an edge which contains* (0,0,1) *and the other two lying on another great circle through* (0,0,1). *Then for large enough* g *there is a horizontal facet on top of* V *if* V *is convex.*

Proof. Suppose that the crystal graph is as in the hypotheses and that V is convex with no facet on top. By corollaries 1 and 2, there can be no facets or continuous families with normals in the edges not containing either (0,0,1) or (0,0,-1) in their closures. But then there can be none in the edge containing (0,0,1) either, since the absence of those other normals implies that the length of any such rulings with normals in that edge would have to be constant, violating the proposition. Thus V is polyhedral near its top, having as its normals the normals of W, and the absence of a facet on top for all g now contradicts minimality, by summary statement 2.

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