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SOME CRYSTALLINE VARIATIONAL TECHNIQUES AND RESULTS

J. E. TAYLOR

The geometric configuration of grain boundaries and surfaces seems to play a significant role in phase transformations and surfaces phenomena in metals. (Metals are usually a mass of small crystals, called grains, which meet each other along grain boundaries; the union of these grain boundaries is often described as being like a soap froth, although this model neglects the orientation-dependance of surface energies caused by the underlying crystalline structure. The word "surface" is often used to designate the boundary between crystals and other phases, such as in catalysis.) Determining the equilibrium (surface energy minimizing) configurations of such interfaces for a given orientation-dependent surface free energy function is additionally an interesting mathematical problem; it reduces in the case of isotropic surface energy to the minimal surface problem. A framework is given here for determining and describing local configurations in the nonisotropic cases. More global results are also given in the case where the Wulff shape (the shape of minimum surface energy for the volume it contains) is a polyhedron.

In what follows, temperature, pressure, and the orientation of each crystalline region are fixed. One of the regions is arbitrarily denoted by I (crystal) and the other by II (matrix); the interface is oriented so that the unit normal points from I to II. The surface free energy function  $\phi$  is then defined on the space of unit vectors in  $\mathbb{R}^3$  (corresponding to oriented normal vectors to the interface). To such a  $\phi$  there is associated a positively oriented convex body

$$W = \{x \in \mathbb{R}^3 : x \cdot n \leq \phi(n) \text{ for each unit vector } n\},$$

the Wulff shape; it is the equilibrium shape of the crystal of fixed volume embedded in the matrix ([13][1][6]). The proof is given again in the appendix to this paper. The central inversion  $WI$  of  $W$  is the equilibrium shape of the matrix of fixed volume embedded in the crystal and has all its normal vectors pointing inwards. (Note: if  $\phi$  is extended by positive homogeneity to a function on  $\mathbb{R}^3$  and if it is then a convex functional, it is the support function of the convex body  $W$ .)

Since any edges and corners of  $W$  are particularly important (the tangent cones at such points are automatically minimizing [6] and so can be used as barriers), it is convenient to describe the Wulff shape in terms of an  $n$ -diagram. The  $n$ -diagram is the decomposition of the unit sphere  $S^2$  induced by the generalized Gauss map of  $\partial W$ . That is, the  $n$ -diagram is a plot on the unit sphere of all the oriented normals to the boundary of the Wulff shape, together with the lines in  $W$ . Tie lines are geodesics connecting the orientations of two planar wedges that meet along a ray in some tangent cone to  $\partial W$ . If such a tangent cone consists of two half planes, it is a tangent cone to  $\partial W$  at a point on an edge of  $W$ , and the normal to the plane containing the corresponding tie line is the direction of the tangent line to that edge of  $W$ . Spherical tie regions represent corners of the Wulff shape, with the regions being tie polygons bounded by tie lines if the tangent cone to the corner is polyhedral. If  $W$  is itself a polyhedron (in which case  $\phi$  will be called crystalline) then the  $n$ -diagram contains only isolated vertices, each representing a facet of  $W$ , connected by tie lines and tie polygons, representing respectively edges and corners of  $W$ . The  $n$ -diagram was introduced and called the crystal graph in that case in [7]. It was introduced in general independently in [2]. A  $W$  and its corresponding  $n$ -diagram are shown in figure 1.

Minimizing surfaces are surfaces of minimum surface free energy compared to all other surfaces spanning the same boundary curve. Physically, one can think of prescribing a boundary curve as a way of isolating part of a larger interface. This way of regarding a prescribed boundary curve is particularly apt for the description of local features of surfaces, such as edges and corners.

One would like to exploit the  $n$ -diagram and as a start to be able to show that the set of normal directions to a minimizing surface should be only vertices of the  $n$ -diagram. However, it is not true: any segment of any plane can be given a varifold structure (sort of an infinitesimal corrugation) so that it becomes minimizing on its boundary. Furthermore, if the normal to the plane is inside a tie region of the  $n$ -diagram, there are uncountably many other minimizing surfaces having the same boundary, and if the normal is inside a tie line, it may be the case that the varifold referred to above is the unique minimum—there may be no classical minimum.

This problem has been handled in several ways. For some simple problems illustrating particular singularities, the solutions can be explicitly determined and shown to have only good normals. In classifying possible minimizing cones (truncated to sit inside the unit ball), we simply look only at those which are classical surfaces and have all of their normals being vertices of the  $n$ -diagram. In looking at more global questions for crystalline surface free energy functions, however, we make further assumptions on  $W$  and on the directions of the tangent lines to the boundary of  $W$ , and we assume that the surface in question is the image of a polyhedral mapping which is minimizing and also volume-maximizing among all minimizing surfaces; in that case, it can be proved that all normal directions

of the surface are vertices of the  $n$ -diagram [ 9 ] .

On the other hand, there are other, very natural situations involving more general integrands which seem to require varifold solutions, so the prejudice in favor of vertices of the  $n$ -diagram should not be allowed to be too strong.

It is easiest to describe cones all of whose normals are vertices of the  $n$ -diagram in terms of "labelled cycles" on the  $n$ -diagram. We define a labelled cycle of length  $k$  to be an oriented closed curve on the  $n$ -diagram, composed of a sequence  $(e_1, \dots, e_k)$  of  $k$  oriented geodesics on  $S^2$ , called edges of the cycle, with each edge being labelled "regular" or "inverse" and with the second endpoint  $n_i$  of  $e_i$  being the first endpoint of  $e_{i+1}$  for  $i = 1, \dots, k$  (here  $e_{k+1} = e_1$ ). To any oriented minimizing cone which is composed of a finite number of wedges whose normals are normals of  $W$  and which is a mapping of the disk, a labelled cycle can be uniquely associated. Its vertices are the normals of the wedges, its edges are the geodesics linking the normals of the wedges (each is in fact either a tie line or its endpoints are vertices of a single tie figure [ 11 ]), its orientation is given by the orientation of the cone, and its edge labels are regular or inverse according to whether a neighborhood of the intersection of the corresponding planar wedges is like that in  $W$  ("normals point away from each other") or that in  $WI$  ("normals point towards each other"). Conversely, to each labelled cycle there corresponds a unique cone  $S$ , constructed as follows. To each edge  $e_i$  there corresponds a "north pole" given by the orientation of  $e_i$  (the end of the thumb in the right hand rule); let  $R_i$  be the line segment from the origin to the north pole if  $e_i$  is labelled inverse and be the line segment from the origin to the south pole if  $e_i$  is labelled regular. The wedge  $P(n_i)$  corresponding to the  $i^{\text{th}}$  vertex  $n_i$  of the cycle is the part of the two-dimensional unit disk with normal  $n_i$  swept out by rotating  $R_i$  into  $R_{i+1}$ . Finally,

$$S = \cup P(n_i).$$

Labelled cycles are used extensively in the description of the results and the proof of the second theorem below. The use of the  $n$ -diagram plus labels is a general tool for describing minimizing polyhedral surfaces, not just cones, and it is exploited in the proof of the last theorem listed below.

The following are some of the results that have been proved :

THEOREM 1 [ 4 ]. For every non-equatorial triangle of tie lines in the  $n$ -diagram, there are minimizing non-self-intersecting saddle-shaped cones consisting of three planar wedges which have the vertices of that triangle as their normals ; their labelled cycles are the triangle, with negative orientation, and with not all three edges labels the same. See figure 2(e). When this surface does not have all its

normals coming from one corner of  $W$ , as in figure 2(e), it provides a counterexample to several expectations previously expressed in the metallurgy literature (see for example [3] and [2] as well as [4]). The proof uses barriers and is given in the appendix.

THEOREM 2 [11][10]. Suppose that  $S$  is a non-self-intersecting cone (truncated to lie in  $S^2$ ) which is minimizing for  $\phi$  and suppose that all of its normals are vertices of the  $n$ -diagram. If all tie polygons of the  $n$ -diagram are tie triangles, then  $S$  consists of one, two, three, four, five, or six planar wedges, as specified in (1)-(10) of the catalog in [11], or it is a modification of one of these types as in (11) of the catalog. If the  $n$ -diagram contains tie polygons that are not tie triangles, but no tie regions that are not tie polygons, then the catalog is still finite, consisting of those basic 11 types and minor variations on them, plus one new modification ((12) of the catalog). Tie regions that are not tie polygons lead to an infinite number of polyhedral cones of type (12), having highly branched generalized Gauss maps. See figure 2 for examples of each of the types. The surfaces of the previous theorem are two of the types, depending on whether a tie triangle is bounded or not. The catalog is given and its implications discussed at length in [11]. It is proved in [10] that it is a complete catalog.

THEOREM 3 [12]. If  $W$  is a cylinder, then there are minimizing surfaces with singular curves containing interior cusps. See figure 3(a). Such cups have also been seen experimentally (see figure 3(b), although the  $W$  in those cases seems not to be a cylinder but to be a ball with six small caps sliced off, leaving planar facets near where the coordinate axes would protrude from the ball.)

THEOREM 4 [1] [8]. Let  $W_g$  be an  $n$ -dimensional region of volume 1 contained in the upper half space and having least total energy (surface energy plus gravitational energy) in a gravitational field with gravity constant  $g$ . If  $g$  is large enough, if  $W_g$  is convex (an open problem!), and if the vertical vector  $(0, \dots, 0, 1)$  is inside a tie region of the  $n$ -diagram for  $W$  (so that  $W$  has a corner on top), then there is a facet on top of  $W_g$  with vertical normal. If  $n = 3$  and the vertical unit vector is part of a tie line on the boundary between two tie regions, then under some conditions on the  $n$ -diagram there must be a facet on top of  $W_g$  and under others there can be no such facet but there must be gravity-induced curvature near the top of  $W_g$ . In either case, if  $\phi$  is not a convex integrand in the region around the vertical unit vector, this facet or curved region must be infinitesimally corrugated—that is,  $W_g$  is not a classical solution but only a varifold solution.

THEOREM 5 [ 9 ]. Suppose that

- (1) W is a polyhedron such that only three facets meet at each corner, each facet of W has an even number of sides with opposite sides being parallel, and the angles between adjacent facets of W are less than  $90^\circ$  ;
- (2) For some positive integer b , B is the union of b disjoint oriented simple closed polyhedral curves, with each line segment of B parallel to some edge of W ;
- (3) For some non-negative integer k ,  $h : M \rightarrow \mathbb{R}^3$  is a polyhedrally parametric mapping of a polyhedral disk with b boundary components and k handles, taking boundary B , and
- (4) h is minimizing among all surfaces taking boundary B and is volume maximizing compared to all other such minima.

Then the number of plane segments in  $h(M)$  is bounded by

$$3N_B/\alpha + (2/\alpha - 1)(b + 2k - 2),$$

where  $N_B$  is the number of line segments in B and  $2\pi\alpha$  is the area of the smallest tie triangle of the n-diagram.

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APPENDIX

Proof of Wulff's construction. Let  $W$  be the Wulff shape for the surface free energy function  $\phi : S^{n-1} \rightarrow R^+$ , as given in the body of this paper. Let  $P$  be any other region with piecewise  $C^1$  boundary and the same volume and center of gravity as  $W$ . We will show

$$\begin{aligned} \phi(\partial P) &\equiv \int_{x \in \partial P} \phi(v_{\partial P}(x)) dH^{n-1}_x \\ &\geq \int_{x \in \partial W} \phi(v_{\partial W}(x)) dH^{n-1}_x \\ &\equiv \phi(\partial W). \end{aligned}$$

By approximation, then, this result holds with only the hypothesis that  $P$  has finite perimeter. The proof that  $W$  is the unique minimum in the strongest possible sense is given in [T6].

The proof (for  $\partial P$  piecewise  $C^1$ ) has three ingredients.

I . There exists a smallest integrand  $\psi$  with the same Wulff shape  $W$  as  $\phi$ . This integrand is a convex function on  $R^n$  (when viewed as a function on hyperplanes rather than their normal directions, it is a semielliptic integrand in the terminology of [F 5.1.2]), and is in fact the support function of the convex body  $W$ .

II .  $\psi(v) = \text{dist}(\partial H^v, \partial(H^v + W))$  for each  $v$  in  $S^{n-1}$ ; here  $H^v$  is the half space whose oriented unit normal is  $v$  and

$$H^v + W = \{x + y : x \in H^v, y \in W\} .$$

III .  $L^n(A+B) \geq (L^n(A)^{1/n} + L^n(B)^{1/n})^n$ , with equality if and only if  $A$  and  $B$  have the same shape (differ only by a translation and/or a homothety), for any sets  $A$  and  $B$  in  $R^n$ . This is the Brunn-Minkowski inequality (see[F 3.2.41]).

As a final bit of notation, for any  $h > 0$  let  $\mu_h : R^n \rightarrow R^n$  be the homothety taking each  $x$  in  $R^n$  to  $hx$ , and let  $v_{\partial P}(x)$  be the exterior unit normal to  $\partial P$  at  $x$  (which is defined for almost all  $x$  in  $\partial P$ ).

We now prove that  $\phi(\partial P) \geq \psi(\partial W)$ .



$$\begin{aligned}
 \phi(\partial P) &\equiv \int_{x \in \partial P} \phi(v_{\partial P}(x)) dH^{n-1} x \\
 &\geq \int_{x \in \partial P} \psi(v_{\partial P}(x)) dH^{n-1} x && \text{(by I)} \\
 &= \int_{x \in \partial P} \lim_{h \rightarrow 0} (1/h) \text{dist}(x, P + \mu_h W) dH^{n-1} x && \text{(by II)} \\
 &= \lim_{h \rightarrow 0} (1/h) (L^n(P + \mu_h W) - L^n(P)) \\
 &\geq \lim_{h \rightarrow 0} (1/h) (n h L^n(W) + (n(n-1)/2) h^2 L^n(W) + \dots + h^n L^n(W)) \\
 &&& \text{(by III and } L^n(P) = L^n(W)) \\
 &= n L^n(W) \\
 &= \lim_{h \rightarrow 0} (1/h) (L^n(W + \mu_h W) - L^n(W)) && \text{(by III)} \\
 &= \int_{x \in \partial W} \psi(v_{\partial W}(x)) dH^{n-1} x && \text{(by II)} \\
 &= \int_{x \in \partial W} \phi(v_{\partial W}(x)) dH^{n-1} x && \text{(by I).}
 \end{aligned}$$

Proof of Theorem 1. The proof uses barriers. Any uniquely minimizing surface can be used as a barrier surface to try to prove that a given surface  $S$  with a given boundary curve is also uniquely minimizing. The idea is that if the given boundary curve lies to one side of the barrier surface, any minimizing surface having the given curve as boundary must also lie to that side of the barrier surface. If  $S$  did cross over the barrier surface, then that part of the barrier surface which would be cut out by  $S$  is uniquely minimizing, and replacing that part of  $S$  with the cut-out of the barrier would decrease the energy. In order to prove by this technique that  $S$  is uniquely minimizing one must be able to pin down every point of  $S$  by barriers from both sides. For the  $S$  specified in the hypotheses of this theorem, two barriers from in front of  $S$  and two from in back of  $S$  suffice.

Suppose that the vertices of the labelled cycle corresponding to  $S$  are  $n_1, n_2, n_3$ , with both edges to  $n_1$  being labelled regular and the other edge of the cycle labelled inverse. Then one barrier from in front is the plane with normal  $n_1$  and another is two half-planes, with normals  $n_2$  and  $n_3$ , meeting in an inverse intersection. Both barriers from in back consist of two half-planes making a regular intersection, one with normals  $n_1$  and  $n_2$  and the other with normals  $n_1$  and  $n_3$ .

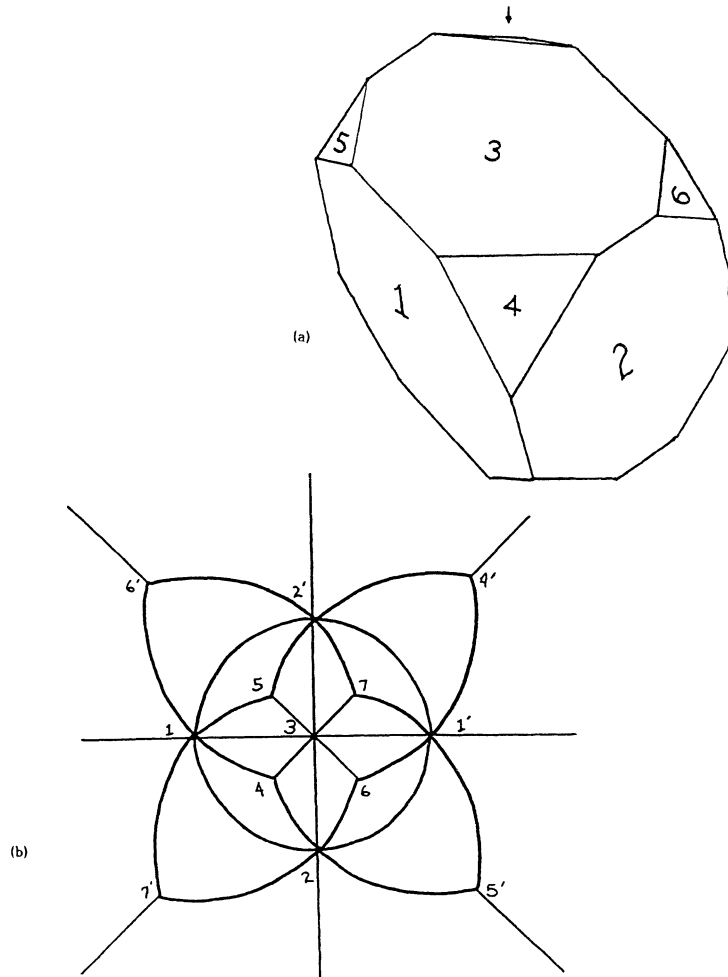


Figure 1. (a) A Wulff shape  $W$ . (b) Stereographic projection from the direction  $v_3$  of the  $n$ -diagram corresponding to this  $W$ .

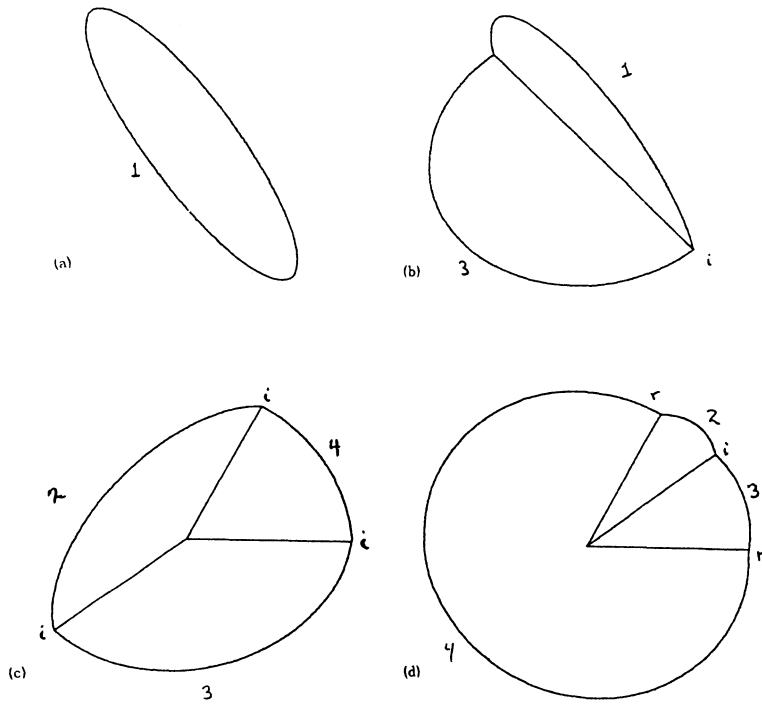
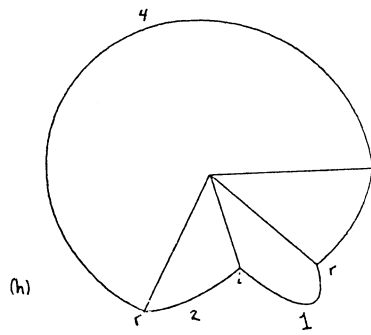
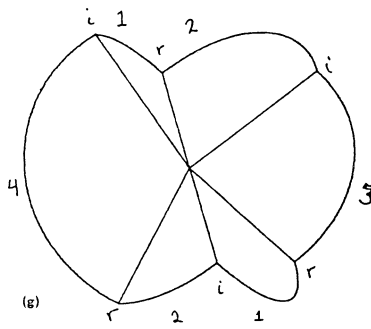
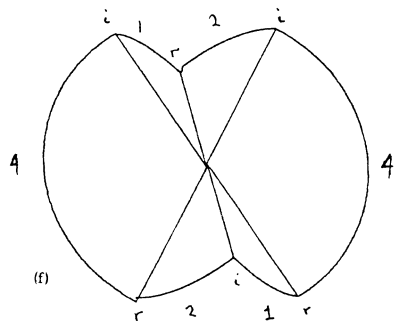
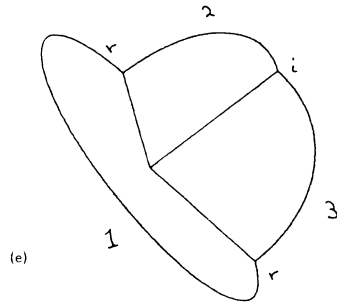
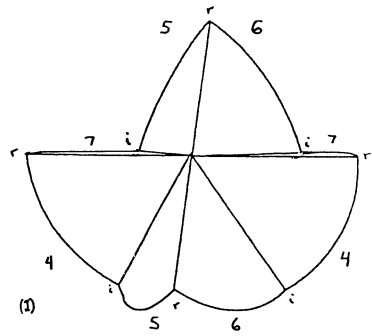
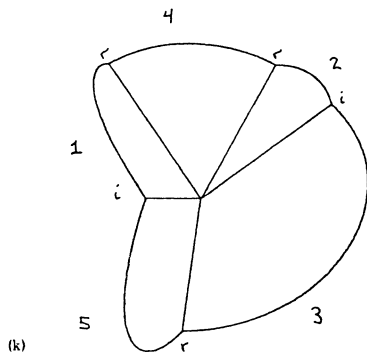
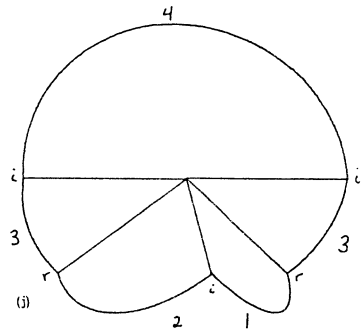
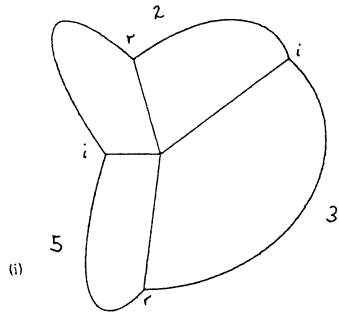


Figure 2. (a) through (l) are examples of cones of types (1) through (12). Cones (a) through (k) are minimizing for the  $W$  shown in figure 1, but (l) requires a different  $W$  such as the octahedron where planes 4,5,6, and 7 meet at a single corner.

CRYSTALLINE VARIATIONAL TECHNIQUES





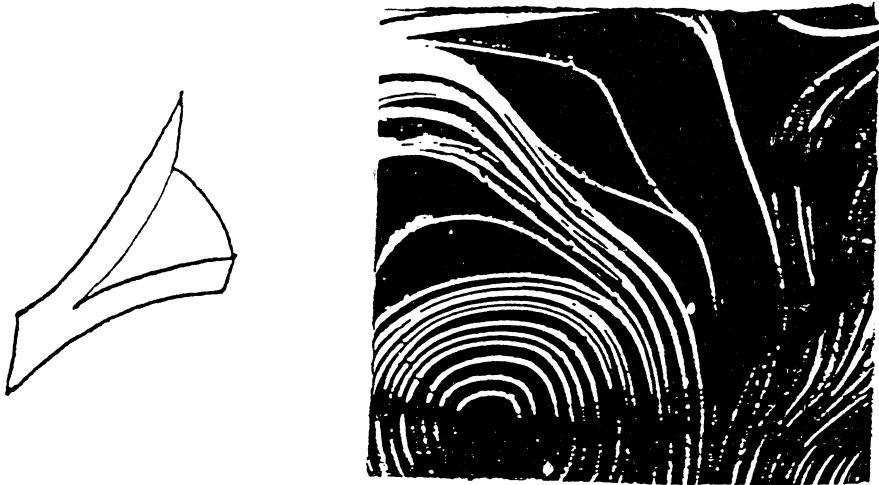


Figure 3. If the Wulff shape  $W$  is a vertical cylinder then a minimizing surface is the surface shown in (a), which has a horizontal ledge terminating in a cusp half way up a vertical wall. In (b) is shown a photograph (magnification 2000X) of a single crystal of a steel whose surface contains cusps ; the  $W$  for this alloy is apparently a ball distorted somewhat toward a cube, with six caps cut off leaving six facets with sharp edges. Photograph courtesy of John L. Walter, G.E. Research and Development Center.

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