A level set approach to the crystalline mean curvature flow

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Understanding the evolution of small crystals has been a challenging problem of material science and mathematical modeling. In this regime, the evolution seems to be governed by the surface energy, whose effects are usually modeled by mean curvature terms. Due to the lattice structure of a typical crystal, the surface energy density is anisotropic. In fact, it is postulated that the surface energy density has certain singularities and such anisotropies are called crystalline. This causes difficulties for the definition of an anisotropic (crystalline) mean curvature, a suitable notion of solutions of the resulting surface evolution problem, and the introduction of an efficient numerical method. In this talk, we discuss some of the recent developments, and in particular focus on the level set method approach to the so-called crystalline mean curvature flow.

1. Crystalline mean curvature flow

Crystalline mean curvature was introduced independently by Angenent and Gurtin [3] and Taylor [33] to model the growth of small crystals, see also [5, 25]. The surfaces of solid and liquid bodies, such as small crystals or water droplets, have a surface energy. This is usually expressed as a surface integral of a surface energy density $\sigma: S^{n-1} \to (0, \infty)$ over the boundary of a set $E \subset \mathbb{R}^n$, representing the body,

$$\mathcal{F}(E) := \int_{\partial E} \sigma(\nu) \, dS,$$

where $\nu : \partial E \to S^{n-1}$ is the unit outer normal of E. n is the dimension, usually 2 or 3. For many materials, especially liquids, σ is a constant on the unit sphere S^{n-1} , given by the surface tension. This surface energy is a manifestation of the fact that the atoms or molecules forming the body have a smaller interaction energy when surrounded by the particles of the same kind. Liquids, typically, do not have any preferred direction in the distribution of particles, and therefore the surface energy density is isotropic.

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Figure 1: Left: Crystal of atoms on a regular lattice. Right: The 1-level set of the associated surface energy density σ and its Wulff shape W.

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The situation is quite different for crystals. Let us give a simplified illustration. If we suppose that the atoms are distributed along the regular square lattice in two dimensions, every atom inside the body has exactly four neighbors with which it creates chemical bonds, see Figure 1. On the surface, however, some of these bonds are broken where a neighbor is missing and the surface energy is proportional to the number of the broken bonds. This number is given in terms of the taxicab (ℓ^1) length of the surface, not the usual Euclidean length. In particular, in this case $\sigma(\nu) \sim ||\nu||_1 := |\nu_1| + |\nu_2|$, where ν is the *macroscopic* unit outer normal. This is the basic motivation of the introduction of nondifferentiable surface energy densities.

For convenience, we will assume that σ is positively one-homogeneously extended from \mathcal{S}^{n-1} to \mathbb{R}^n as

$$\sigma(p) = |p|\sigma(\frac{p}{|p|}), \qquad p \in \mathbb{R}^n \setminus \{0\},$$

 $\sigma(0) = 0$, where $|p| := (\sum_i |p_i|^2)^{1/2}$ is the usual Euclidean norm.

If σ is convex on \mathbb{R}^n and $\sigma(p) > 0$ for all $p \in \mathbb{R}^n \setminus \{0\}$, we call it an *anisotropy*. We are in particular interested in anisotropies σ that are piece-wise linear, such as the ℓ^1 -norm $\sigma(p) = \|p\|_1 := \sum_i |p_i|$. Such anisotropies will be called **crystalline anisotropies**.

The optimal shape of the crystal, that is, the shape with minimal surface energy for a given volume, is a translation and scaling of the Wulff shape

$$\mathcal{W} := \{ x : x \cdot p \le \sigma(p), \ p \in \mathbb{R}^n \}.$$

The evolution $\{E_t\}_{t\geq 0}$ of the body driven by the dissipation of the surface energy then leads to a formal gradient flow

$$\beta(\nu)V = \kappa_{\sigma} + f \qquad \text{on } \partial E_t,$$
(1.1)

where V is the normal velocity of the surface ∂E_t , f = f(x, t) is a given external force, and $\beta : \mathcal{S}^{n-1} \to (0, \infty)$ is a *mobility*. Finally, $-\kappa_{\sigma}$ is the first variation of the surface energy \mathcal{F} at E_t . κ_{σ} is usually called the anisotropic mean curvature of the surface.

If $\sigma \in C^2(\mathbb{R}^n \setminus \{0\})$ and $\{p : \sigma(p) < 1\}$ is strictly convex, then it is well-known [17] that the anisotropic mean curvature can be evaluated as

$$\kappa_{\sigma} = -\operatorname{div}_{\partial E}(\nabla \sigma)(\nu)_{E}$$

where $\operatorname{div}_{\partial E}$ is the surface divergence on ∂E .

When σ is crystalline, the situation is significantly more complicated. In particular, even if ∂E is smooth, $\nabla \sigma(\nu)$ will be discontinuous (or not even defined) on some parts of the surface. Therefore κ_{σ} might not be defined, or might not be a function.

Instead, following for example [5], we define the subdifferential of σ as

$$\partial \sigma(p) := \{ \xi \in \mathbb{R}^n : \sigma(p+h) - \sigma(p) \ge \xi \cdot h, \ h \in \mathbb{R}^n \},\$$

where $\xi \cdot h$ is the usual inner product on \mathbb{R}^n . Note that $\partial \sigma(p)$ is a nonempty compact convex subset of \mathbb{R}^n . We replace $\nabla \sigma(\nu)$ by a vector field $z : \partial E \to \mathbb{R}^n$, usually called a Cahn-Hoffman vector field, that is a selection of $\partial \sigma(\nu(x))$ on ∂E , that is, $z(x) \in \partial \sigma(\nu(x)), x \in \partial E$. However, now there are multiple choices of z which potentially lead to different values of $\kappa_{\sigma} = -\operatorname{div}_{\partial E} z$. It turns out that a reasonable choice is a vector field z_{\min} that minimizes $\|-\operatorname{div}_{\partial E} z + f\|_{L^2(\partial E)}$. The crystalline (mean) curvature is then defined as

$$\kappa_{\sigma} := -\operatorname{div}_{\partial E}(z_{\min}).$$

Such a choice is motivated by the standard theory of monotone operators by [10, 27]. Furthermore, since the Euler-Lagrange equation of the minimization problem is $\nabla(-\operatorname{div}_{\partial E} z + f) = 0$, this choice yields $\kappa_{\sigma} + f$ that is constant, if possible, on flat parts, or facets, of the crystal parallel to the flat parts of the Wulff shape \mathcal{W} . Therefore facets are usually preserved during the evolution, as expected. However, κ_{σ} might be even discontinuous on facets, and then facet breaking or bending occurs [8] and Figure 4. This poses a serious difficulty for introducing a suitable notion of solutions for this problem. Since κ_{σ} is itself given as a solution of a minimization problem, it is in general difficult to evaluate it, except in special circumstances. Moreover, κ_{σ} is a nonlocal quantity on the facets of the crystal as the following example shows.

Example. Consider the cubic anisotropy $\sigma(p) = \|p\|_1 := \sum_{i=1}^n |p_i|$ and suppose that the initial shape is the cube centered at 0 with side-length $L_0 > 0$, $\beta \equiv 1$. Let us try to find $\{E_t\}_{t\geq 0}$. It is not difficult to see that for a cube $Q_L = (-\frac{L}{2}, \frac{L}{2})^n$, L > 0, the vector field $z(x) = \frac{x}{\sigma^\circ(x)}$ is a Cahn-Hoffman vector field on ∂Q_L , where $\sigma^\circ(x) := \sup \{x \cdot p : \sigma(p) \leq 1\}$. σ° is the convex polar of σ and it is the dual norm of σ , $\sigma^\circ(x) = \|x\|_{\infty} := \max_{1\leq i\leq n} |x_i|$. In particular, $\sigma^0(x) = \frac{L}{2}$ on ∂Q_L . Therefore $\operatorname{div}_{\partial Q_L} z = \frac{2}{L}(n-1)$. Since it is a constant on the facets, z actually minimizes $\|-\operatorname{div} z\|_{L^2(\partial Q_L)}$ among all Cahn-Hoffman vector fields, and therefore $\kappa_{\sigma} = -\frac{2}{L}(n-1)$ if $f \equiv \operatorname{const}$. We deduce that, if $\frac{2}{L_0}(n-1) \geq f \equiv \operatorname{const}$ so that solution is shrinking, the solution of (1.1) is $\{E_t\}_{t\geq 0}$, $E_t = Q_{L(t)}$, where $L(0) = L_0$ and $L' = -\frac{2}{L}(n-1) + f$. When f = 0, the unique solution is $L(t) = \sqrt{L_0^2 - 4(n-1)t}$. At time $t_1 := \frac{L_0^2}{4(n-1)}$ the cube vanishes.

If the forcing term f is strong enough, the crystal will grow. However, it will only stay a cube as long as the velocity of corners is less than f. If the speed of the corners is bigger, the corners will round up, as can be easily seen by the comparison principle. See for example [21] and references therein.

Introducing a notion of solutions for (1.1) with the crystalline anisotropy have been a challenging problem. In two dimensions, if f is constant on facets, the situation is somewhat simpler since κ_{σ} is constant on facets of the crystal parallel to the facets of the Wulff shape \mathcal{W} . Therefore if the initial shape is a polygon with edges parallel to edges of the Wulff shape, the facets will move without breaking or bending. Their evolution can be tracked by the crystalline algorithm [33], which also yields efficient numerical methods. However, these methods cannot treat evolutions that are not strictly faceted.

In three dimensions, the situation is significantly more complicated by the possible bending or breaking of facets. There is an extensive number of publications that is beyond the scope of this abstract, for instance [6–9], and [5] for an introduction to the topic and references. Recently, Chambolle, Morini and Ponsiglione [12] introduced a well-posed notion of solutions for the particular velocity law $V = \sigma(\nu)\kappa_{\sigma}$. Independently, Y. Giga and the author introduced a well-posed notion of viscosity solutions for the level set formulation of (1.1) in the full generality, but constant f, for bounded crystals, see Section 2.

As for the available numerical results, published results concerning the purely crystalline anisotropy so far seem to only treat the two dimensional evolution. However, the algorithm proposed in [11, 29] generalizes naturally to three dimensions, and can easily accommodate a general external force as explained in Section 3. We present some of the results of this implementation below. Let us also mention the interesting three dimensional results of [4], who develop a finite element method for the Stefan problem with Gibbs-Thomson law that features an almost-crystalline, but still smooth, anisotropic curvature. However, their method does not seem to be able to treat topological changes. See also [16] for a survey of various numerical approaches.

2. Level set method

The level set method for the mean curvature flow was introduced and developed in [13, 15, 30]. The basic idea is to introduce an auxiliary function $u : \mathbb{R}^n \times [0, \infty)$, whose evolution of every level set $\{\{x \in \mathbb{R}^n : u(x, t) < c\}\}_{t \geq 0}, c \in \mathbb{R}$, satisfies the velocity law (1.1). It is easy to see [17] that in this case

$$V = -\frac{u_t}{|\nabla u|}, \qquad \nu = \frac{\nabla u}{|\nabla u|}, \qquad \text{and} \qquad \kappa_\sigma = -\operatorname{div}[(\nabla \sigma)(\nabla u)].$$

Therefore u formally satisfies the equation

$$-\beta \left(\frac{\nabla u}{|\nabla u|}\right) \frac{u_t}{|\nabla u|} = -\operatorname{div}[(\nabla \sigma)(\nabla u)] + f \quad \text{in } \mathbb{R}^n \times 0.$$
(2.1)

If σ is a crystalline anisotropy, $\nabla \sigma$ might be discontinuous and therefore the differential operator on the right-hand side is very singular. In fact, it is a nonlocal operator on flat parts of the surface of the crystal in the directions of the flat parts of the Wulff shape. Therefore this equation does not fit withing the classical framework of viscosity solutions for geometric equations [13, 15]. The extension of the viscosity theory to (2.1) had been a challenging open problem. In one dimension, which also covers two-dimensional crystals, the theory was developed by M.-H. Giga, Y. Giga, Rybka and others [18–20]. Y. Giga and the author recently introduced a new notion of viscosity solutions for (2.1) with f independent of the space variable that applies to the crystalline anisotropy [22, 23]. This notion is well-posed for bounded crystals and stable with respect to a regularization of the anisotropy, that is, with respect to the approximation of the crystalline curvature by smooth anisotropic curvatures. The main idea is the suitable interpretation of the operator div $[(\nabla \sigma)(\nabla u)]$ as the divergence of a minimizing Cahn-Hoffman vector field $z \in \partial \sigma(\nabla u)$, which allows us to connect this to the theory of monotone operators of [10, 27].

3. The algorithm

An efficient method for the mean curvature flow (1.1) is based on a minimizing movement formulation due to [11], that can be efficiently solved by a split Bregman iteration proposed by [29]. Suppose that $\Omega \subset \mathbb{R}^n$ is a bounded domain and that the evolving set is contained in Ω .

The insight of Chambolle is to formulate the minimizing scheme of Almgren, Taylor and Wang [2] in terms of the signed distance function, so that the evolving set is its level set. In [11], he proposed the time discretization by the minimization problem (in [11] $f \equiv 0$)

$$v_{m+1} \leftarrow \underset{v}{\operatorname{arg\,min}} \left(\frac{1}{2h} \left\| v - w_m \right\|^2 + \int_{\Omega} \sigma(Dv) \, dx - \langle v, f \rangle \right), \tag{3.1}$$

where h > 0 is a chosen time step and w_m is the signed distance function of the set at the previous time step m, induced by the metric given by the mobility β . The minimization is performed over all $v \in L^2(\Omega)$, and $\|\cdot\|$ and $\langle \cdot, \cdot \rangle$ are the $L^2(\Omega)$ -norm and inner product, respectively. The total variation energy $\int_{\Omega} \sigma(Dv) dx$ is defined as the lower semicontinuous envelope of $v \mapsto \int_{\Omega} \sigma(\nabla v) dx$ for v in the Sobolev space $W^{1,1}(\Omega)$. Note that (3.1) is the resolvent problem for the total variation energy with parameter $\frac{1}{h}$. In other words, it is the implicit Euler discretization of the total variation flow. Since $|\nabla v| \sim |\nabla w| = 1$, we see that $\frac{v-w}{h} \sim V$.

The full algorithm for the minimizing movements discretization E_m , m = 0, 1, 2, ...at time steps $t_m = mh$ reads: Set E_0 as the initial data and then iteratively for m = 0, ... do

$$w_m \leftarrow \operatorname{signdist}_{\beta} E_m$$

$$v_{m+1} \leftarrow \operatorname{arg\,min}_{v} \left(\frac{\mu}{2} \|v - w_m\|^2 + \|\sigma(\nabla v)\|_1 - \langle f, v \rangle\right), \qquad (3.2)$$

$$E_{m+1} \leftarrow \{v_{m+1} < 0\},$$

where $\mu = \frac{1}{h}$, and f is a given source, and we write $\|\sigma(\nabla v)\|_1 = \int_{\Omega} \sigma(Dv) dx$. Note that the minimization is equivalent to the minimization of $\frac{\mu}{2} \|v - (w_m + \mu^{-1}f)\|^2 + \|\sigma(\nabla v)\|_1$. The signed distance function must correspond to the anisotropy β . If $\beta \equiv 1$, it is just the standard signed distance function induced by the Euclidean metric,

signdist
$$E_m(x) := \begin{cases} \operatorname{dist}(x, \partial E_m), & x \notin E_m, \\ -\operatorname{dist}(x, \partial E_m), & x \in E_m. \end{cases}$$

As $h \to 0$, the evolution will converge to a continuous evolution $\{E_t\}_{t\geq 0}$, see [11]. In the crystalline anisotropy case, it is known that in two dimensions this evolution is given by the unique viscosity solution [26]. It is not clear at the moment if this also holds in three dimensions for viscosity solutions introduced in [22, 23], although we expect it to be the case.

It might seem that the minimization problem in (3.2) is rather difficult for numerical computation, mainly due to the non-differentiable second term. In particular, the standard minimization methods like conjugate gradients or Newton iteration are poorly suited. For this reason, Chambolle proposed an iterative algorithm in [11]. More recently, it was recognized in [29] that the minimization problem can be addressed by the so-called proximal algorithms [28], the alternative direction method of multipliers (ADMM) or the split Bregman method [24]. To find the minimizer v of $\frac{\mu}{2} ||v - u||^2 + ||\sigma(\nabla v)||_1$, we choose $\lambda > 0$, set $b_0 = d_0 = 0$ and then iterate for $k = 0, 1, \ldots$

$$v_{k+1} \leftarrow \arg\min_{v} \frac{\mu}{2} \|v - u\|^2 + \frac{\lambda}{2} \|d_k - \nabla v - b_k\|^2,$$
 (3.3)

$$d_{k+1} \leftarrow \arg\min_{d} \|\sigma(d)\|_{1} + \frac{\lambda}{2} \|d - \nabla v_{k+1} - b_{k}\|^{2}, \qquad (3.4)$$

$$b_{k+1} \leftarrow b_k + \nabla v_{k+1} - d_{k+1},$$
 (3.5)

until some stopping condition is reached, typically when $||v_{k+1} - v_k||_2$ is sufficiently small. Heuristically, this scheme introduces a new gradient variable d, and then enforces the constraint $d = \nabla v$ by a quadratic penalty. Since we are minimizing a sum of convex terms over two variables, the problems can be decoupled into (3.3) and (3.4). (3.5) is called a Bregman iteration, and it helps to enforce the constraint *exactly*. Note that when convergence is achieved, (3.5) implies $d = \nabla v$. For a detailed discussion of motivation, convergence and other properties, see [24].

The advantage of this iteration process is the simplicity of the subproblems. The first minimization problem (3.3) is equivalent to finding the solution v of

$$(\mu - \lambda \Delta)v = \mu u + \lambda \operatorname{div}(b_k - d_k) \quad \text{in } \Omega, \tag{3.6}$$

with an appropriate boundary condition, for instance Neumann. It is not necessary to solve it accurately, so one or two Gauss-Seidel iterations are enough [24].

To find a numerical solution of Chambolle's algorithm, we assume that $\Omega = (-\frac{1}{2}, \frac{1}{2})^n$ is a cube and use the finite difference method to discretize (3.2). In particular, we represent v, d, b by their values on the lattice $k\mathbb{Z}^n \cap \overline{\Omega}$, where $k = \frac{1}{M}$, $M \in \mathbb{N}$, is the space discretization step. The elliptic problem (3.6) is solved by the Gauss-Seidel iteration for the standard 5-point fixed difference scheme with zero Neumann boundary condition.

The minimization problem (3.4) for d in the discrete case completely decouples at each node. Then, for each node i the minimum $d_{k+1,i}$ is the so-called shrink operator [24]

$$d_{k+1,i} = \operatorname{shrink}_{\sigma}((\nabla v_{k+1} + b_k)_i, 1/\lambda).$$
(3.7)

Note that the shrink operator can be expressed using the orthogonal projection on the Wulff shape \mathcal{W} of σ [29],

$$\operatorname{shrink}_{\sigma}(\xi, 1/\lambda) := (I - P_{W/\lambda})(\xi)$$

In typical cases of isotropic, cubic and hexagonal anisotropies, that is, when the Wulff shape \mathcal{W} is a sphere, a cube or a hexagonal prism, respectively, the orthogonal projection is very simple. More general Wulff shapes can be handled by the method proposed in [29].

It is interesting to relate the Bregman iterate b to the Cahn-Hoffman vector field in the definition of the anisotropic (crystalline) mean curvature. In particular, for a node i, if convergence is achieved, (3.7) yields $d_i = \operatorname{shrink}(d_i + b_i, 1/\lambda)$ and we have $b_i = P_{\mathcal{W}/\lambda}(d_i + b_i)$. From the last equality, we see that either $d_i = 0$, but then $\lambda b_i \in \mathcal{W}$, or $d_i \neq 0$, but then $\lambda b_i \in \partial \mathcal{W}$ and d_i is a normal of $\partial \mathcal{W}$ at λb_i . In other words, $\lambda b_i \in \partial \sigma(d_i)$. From (3.6) we deduce that $\frac{v-u}{h} = \lambda \operatorname{div} b$. Hence λb is the discrete Cahn-Hoffman vector field for the resolvent problem (3.1).

4. Redistance

At each time step in the algorithm (3.2), the signed distance function to the 0-level set of the solution of the minimization problem, $\operatorname{signdist}_{\beta} \{v_m < 0\}$, has to be recomputed. This is sometimes referred to as *redistance*. This problem amounts to solving the (anisotropic) eikonal equation $|\nabla w|_{\beta} = 1$ with boundary data w = 0 on ∂E . There are various efficient methods for doing this, including an iteration scheme [32], as well as more direct algorithms like the fast marching method [31] or the fast sweeping method [34]. We choose the fast sweeping method due to its simplicity and efficiency on the modern hardware, in particular the cache locality.

The boundary ∂E is given as the 0-level set of a function v with discrete values on a regular grid. Unfortunately, in general the 0-level set of the resulting approximation w of the signed distance function will be different from the 0-level set of the original function v. The fast marching and fast sweeping methods require an initialization step, where the distance function is assigned at grid points that are direct neighbors of the 0-level set of v. A special care must be taken so that the interface is not moved unnecessarily, as these effects might quickly accumulate over a series of consecutive time steps. In particular, at points where the surface should not move, a typical case for non-convex and non-concave facets, this unwanted effect might dominate the evolution.

There are a few standard schemes to initialize the nearby values in the literature, by analyzing the intersection of the level set with the grid lines [1, 11]. However, they do not seem to produce the correct value of the distance function even if the level set is flat, which is a common situation in the crystalline mean curvature flow. Furthermore, the generalization to three dimensions seems unnecessarily complicated.

We choose a naive method that appears to be superior in our case, is very simple to implement in an arbitrary dimension, and that computes the *exact* signed distance function in a neighborhood of the flat facets. Let us assume that $\beta \equiv 1$. The idea is to split the squares or the cubes of the uniform grid into two right triangles or six tetrahedra, respectively, and suppose that v is affine on each of them. This is very much in the spirit of the marching tetrahedra method [14]. Then for all elements that the 0-level set intersects, that is, on which v changes sign, we set the initial value of the signed distance function at each vertex of the element to be the value of v normalized by the norm of the gradient of the affine function given by v on the element. If a given grid node is a vertex of multiple elements with 0-level set in them, we set the initial value to be the minimum over all the elements. To be more explicit, suppose that v_i , w_i , $i = 1, \ldots, N$ are the values at the grid nodes x_i , and \mathcal{T}_j , $j = 1, \ldots, K$ are the elements on which v changes sign. We initialize w_i to

$$w_i = (\operatorname{sign} v_i) \min_{\substack{1 \le j \le K \\ x_i \in \partial \mathcal{T}_j}} \frac{|v_i|}{\left| \nabla v |_{\mathcal{T}_j} \right|}$$

where the minimum is defined as $+\infty$ if it is over an empty set. This initialization method is as second order accurate, $O(k^2)$, near smooth surface, in contrast to the first order accuracy of the initialization in [1,11]. Moreover, the unwanted artifacts caused by redistance seem to be reduced, see Figure 2.

After this initialization step, we perform the 2^n sweeps of the fast sweeping method [34].

5. Numerical results

We present a few simple numerical results for an illustration based on our implementation of the above algorithm in the Rust programming language. The domain is always taken to be $\Omega = (-\frac{1}{2}, \frac{1}{2})^n$ and $\lambda = 2\mu$ in (3.3), (3.4). The stopping condition is chosen as $\|v_{k+1} - v_k\|_{\ell^2} < 3 \times 10^{-4} M^{\alpha}$, where $\alpha = 0$ for n = 2 and $\alpha = \frac{1}{2}$ for n = 3, and $\|\cdot\|_{\ell^2}$ is the discrete ℓ^2 -norm. We use M = 64 in n = 2 and M = 256 for n = 3. The performance for n = 3 is ~ 1min/timestep on a single core of i7-4770K.

Various optimizations, such as performing the computation only in a small neighborhood of the level set to significantly reduce the computational complexity, as well as the coupling of the curvature flow with the heat equation via the Gibbs-Thomson relation are under investigation.



Figure 2: Flow with cubic (left) and hexagonal (right) anisotropies: $h = 2.5 \times 10^{-4}$, M = 64, plot step 0.004. Even at this relatively low resolution, artifacts caused by redistance are not apparent.



Figure 3: Left: A triangular anisotropy demonstrates a topological change in 2D for non-even anisotropies. Right: Cubic anisotropy with a non-constant source—a multiple of the standard mollifier with radius 0.2 located at (0.2, 0).



Figure 4: Facet breaking example in 3D [8] at three selected times—L-shaped facets break into rectangular facets. The rightmost figure shows a detail of the facet bending and rounding of a corner in the third figure.



Figure 5: Topological change in 3D with a hexagonal anisotropy—a pinch-off of an initial dumbbell shape.

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