ON A THEORY OF FORMATION OF SNOW CRYSTAL

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There are developed celebrated theories to explain why snow crystal is of hexagonal shape and how it grows by K. HIGUCHI, M. KOMABAYASHI, T. KURODA, A. ONO and U. NAKAYA.

The main framework in them is on one hand to reduce the problem to the non homogeneity of water molecule and on the other hand to describe the growth by the GIBBS THOMPSON type differential equation, assuming that the growth rate is proportional to the vapor density and that the vapor density on the boundary of the crystal is a linear function of the curvature of the boundary.

Computer simulations by KOMABAYASHI (also by A. SHIKATA though not published) based on these theories yield essentially figures of hexagon only with needles attached on the vertices and hardly give that with branching, which is also common among snow crystals.

Instead of starting from given equations, we start with several facts obtained by experiments and we investigate what type of equations is necessary to have the branching, in order to see what is the mechanism for it.

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In what follows we restrict ourselves only for two dimensional theory of crystal formation.

We assume first that the growth rate of the crystal is governed universally by a function w defined on the boundary of the crystal, that is, denoting by n(P) the outer normal to the crystal on its edge at P, we have

$$dn/dt = w$$

on the edge of the crystal universally.

Let bd(B) denote the boundary of a domain B and let ch(B) denote the characteristic function of B, then the universality above suggests us that we need to have a universal differential operator D on the mollified characteristic function g*ch(B) for a suitable mollifier g so that the function w on the edge is written as

$$w = D(g*ch(B)), \text{ for any } B,$$

moreover, the operator should be a function of first and second order derivatives and naturally be independent of the choice of the coordinate, here we assume that the function is a polynomial function.

Though a little rough, the reasoning is as follows: Suppose we are given a homogeneous crystal B, then it is represented by the characteristic function in the function space on the plane, maybe mollified by a mollifier from experimental reason. Since the function w for this crystal is a function on the edge of the crystal, the operator to make correspond w to g*ch(B) in the function space should

be a differential operator.   On the other hand, if there

exists another crystal C in a neighborhood of B, the effect

of the crystal C on the growth of the crystal B is known

to be always non positive independent of the distance and of

the shape of C, therefore D(g) should have only negative zone

around the edge bd(B) of B for a sufficiently large class of

the mollifiers g, yielding that the operator D is a function

of at most second order derivatives.

We determine explicitly above class of operators,

which may describe the growth rate on the edge.

For   the   determination   we first remark that the

independence of the choice of the coordinate is equivalent to

the invariance under the action of the orthogonal group and

that the invariant differential operator in first and second

order derivatives is of the form H(L,det,grad), where det,

grad denotes the operator given by

$$det(f) = (f_{xy})^2 - 4 (f_{xx})(f_{yy}) \, ,$$

$$grad(f) = (f_x)^2 + (f_y)^2$$

respectively, and L denotes the Laplacian in xy coordinate.

In fact, when we denote by X,Y,Z ; U,V the second

and first derivatives

$$X(f) = f_{xx} \quad , \quad Y(f) = f_{xy} \quad , \quad Z(f) = f_{yy} \quad ,$$

$$U(f) = f_x \quad , \quad V(f) = f_y$$

respectively, then the invariance of an operator expressed as
a function $H(X,Y,Z;U,V)$ of X,Y,Z ; U,V implies

$$2Y(H_X + H_Z) + (-X + Z)H_Y = 0 \quad ----(1)$$

$$V H_U - U H_V = 0 \quad ----(2)$$

Rewriting (2) by the polar coordinate R,A :
$$U = R \cos A, \quad V = R \sin A,$$
we have that

$$H_A = 0$$

indicating that H is only a function of grad on its first order
part. By a rotation of 45 degree of XZ coordinate around Y
axis in XYZ space, (1) is reduced to an equation of type (2)
and therefore we see that H is a function in L and det on its
second order part, in a similar way.

Consider a homogeneous crystal having its edge on
x axis, then the operator det vanishes away on the edge for
any mollifier g, thus we throw det away from the variable
in H. By a similar argument, we throw grad away too.

Thus we may conclude that the growth rate operator D
is obtained in a form $H(L)$ of a function of the Laplacian L.

The computer simulation using the growth equation
$$dn/dt = H(L) (g*ch)$$
with the simple characteristic function does not give the
branching type crystal. This might be explained also from

experimental reason that the growing crystal can never be homogeneous and can not be represented by the characteristic function.

In order to meet the transient stage, we then introduce a status function s and a effect function E: the status function s(B)(P,t) is a function in the position P and in time t defined for a crystal B, which represents the status of B determined by the effect of existing crystals, and the effect function E(B,C)(P,t) is a function in t and P which evaluates the effect of a crystal C on B and is determined by s(B) and s(C).

We may assume that s, E and the characteristic function are related by

$$ds/dt = E, \quad s(B)(0) = ch(B).$$

In a similar way as for the growth rate operator, we can deduce that the effect E(B,C) of C on B is obtained from the action of a differential operator on the functions s(B),s(C). For the determination of the effect operator, we can assume again from experiments that it is additive, thus the possible type of operators is much more restricted than in the case of the growth rate operator and a similar argument reduces it to that which is expressed by a linear function K of the Laplacian. Hence we have that

$$E(B,C)(P,t) = K(L)(s(B) + s(C))(P,t).$$

With the preparations above, we consider the growing

process of a crystal.

Also from practical reason, we assume that the process is stepwise, that is, we assume a sequence of pairs $B(i)$, $s(i)(P)$ $(i=0,1,..)$ of crystals and status functions in discrete time is given successively in such a way that for $i=0$

$$B(0) = B, \quad s(0) = g*ch(B)$$

and that the normal vector to $bd(B(i))$ of the length

$$eH(L)(s(i))$$

for a short time unit e determines the next crystal

$$B(i+1) = B(i) + C(i)$$

and finally that

$$s(i+1)(P) = s(i)(P) + eK(L)(s(i) + g*ch(C(i)))$$

gives the status function $s(i+1)$ for $B(i+1)$.

Suppose we have a growth of needle type up to $i=m$ then we may consider i is topologically equivalent to the length of the needle and the growth rate $H(L)s(i)$ is monotone on each side of the needle. This situation may correspond to the case of codimension zero catastrophy of R. THOM, thus we see that the higher catastrophy may be necessary for the branching.

Observation tells us that both needle and branch grows at the same time, therefore we see that $H(L)s(i)$ has to increase first till a maximum, decrease next to a minimum and increase again towards the end of the needle so as to

give a branch at the maximum point, while the growth is
suppressed at the minimum.   The situation may correspond
to the catastrophy of codimension one.

On the other hand, though a little rough again, we see
that the function s(i)(P) increases first and after maximum
decreases until the end of the needle, and its Laplacian
behaves in the other way, provided that the needle growth is
not quick.   In fact, the equation for the status function is
nothing but the heat equation in the limit, because K(L) is
equivalent to the Laplacian itself, therefore we may use the
fundamental solution u(t,x) of the heat equation to investigate
the process, which is interpreted as successive attaching of
unit crystals of a certain temperature.   We see that s(i) and
the second derivative of s(i) in P is a sum of the terms

$$2ve \ u(je, ve(j-x)),$$

$$-v^3 e^2 j^{-1} u(je, ve(j-x)) \ (approximately)$$

for j=1 to i, respectively, where v is the speed of the growth
in needle direction, assumed to be constant and small.   Thus
we see the first derivative is monotone and positive at one end
and negative at the other end of the needle, also by a similar
argument, we have roughly the conclusion.

Hence we see that the growth rate H(L)s for branching
is hardly realized by L(s) only, which can be monotone or have

only one minimum at most, depending on conditions. On the contrary, we see that $H(L)$ should contain at least second order term of $L(s)$ or a term obtained by a multiplication of at least first order term of $s(i)$ to $L(s)$, for the branching growth.

For the simulation purpose this is sufficient and for finding the mechanism problem this, especially the latter possibility suggests us that the diffusion described by the Laplacian multiplied by a non linear term, which may be interpreted as the diffusion efficiency, plays the main role to give the branching, indicating that the heat diffusion, for instance, decides the shape of snow crystal in a generic sense.

We admit the present note is a little rough and we sincerely hope to publish a completed version in near future unified by the idea of the superpotential.