ADDENDUM to Predicting Crystal Growth by Spiral Motion

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Snyder and Doherty[1] used the following equations to calculate the rotation time of a spiral regardless of whether an edge disappears during the first rotation, or whether no edges disappear:

$$\tau = \sum_{i=1}^{N} \tau_{i+1}^{rot} \tag{1}$$

where

$$\tau_{i+1}^{rot} = \frac{l_{i+1,c} \sin(\alpha_{i,i+1})}{v_i} \tag{2}$$

and where τ_{i+1}^{rot} is the time take for edge i+1 to reach its critical length, $l_{i+1,c}$, and where alpha is the outer angle between two edges, as seen in Figure 1.

However, in the case when edge i disappears during the first rotation, they throw away that disappearing edge and use the closest previous edge that has not disappeared, such that they completely ignore edge i when using eq 1. That is to say, $\tau_i^{rot} = 0$ and the value of τ_{i+1}^{rot} becomes:

$$\tau_{i+1}^{rot} = \frac{l_{i+1,c} \sin(\alpha_{i-1,i+1})}{v_{i-1}} \tag{3}$$

Therefore, if edge i disappears, Snyder and Doherty's approach tells us that

$$\tau_i^{rot} + \tau_{i+1}^{rot} = \frac{l_{i+1,c} \sin(\alpha_{i-1,i+1})}{v_{i-1}} \tag{4}$$

It may not seem logical to completely throw away edge i if it disappears, when we know that part of edge i+1 will grow before edge i disappears. Below we derive an equation for the rotation time of a spiral, assuming that

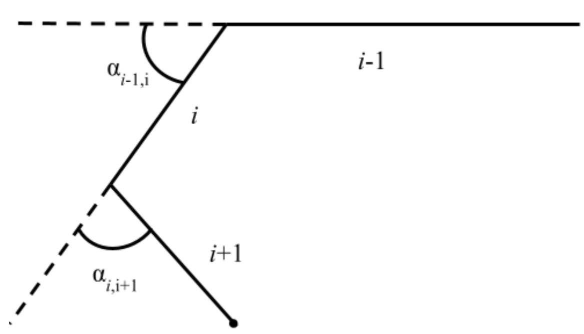

Figure 1: α is the outer angle between two edges.

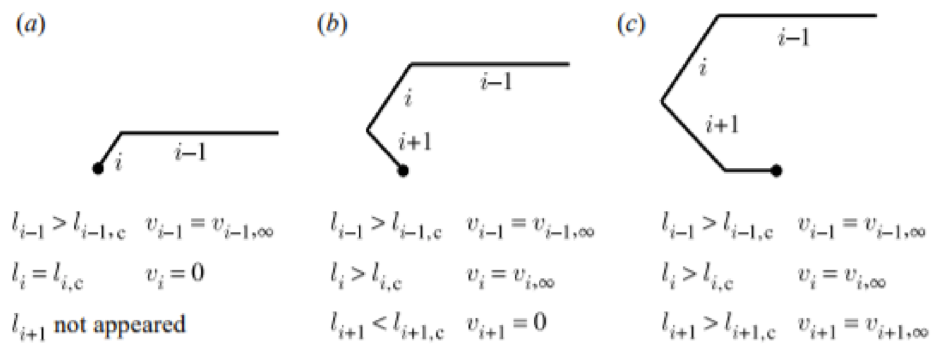

Figure 2: The three stages of the growth of an edge, taken from Snyder and Doherty[1]. (a) Stage 1, the length of edge i is increasing due to the motion of edge i-1. (b) Stage 2, edges i and i-1 are moving, and the length edge i+1 is increasing due to the motion of edge i. (c) Stage 3, all of the edges i-1, i, and i+1 are moving.

edge i disappears, and that edges $i+1$ and $i-1$ have not disappeared. The result of this investigation is a proof that the two approaches are identical.

There are three stages in the growth of edge i, depicted in Figure 2. The tangential velocity of edge i varies depending on the stage that the edge is in. The general equation for the tangential velocity of edge i is as follows (eq 2.6 from Snyder and Doherty[1]):

$$v_i^t = \frac{v_{i+1} - v_i \cos(\alpha_{i,i+1})}{\sin(\alpha_{i,i+1})} + \frac{v_{i-1} - v_i \cos(\alpha_{i-1,i})}{\sin(\alpha_{i-1,i})} \tag{5}$$

Using eq 5, the tangential velocity in stages 1 and 2 can be simplified by knowing when the values of v_i and v_{i+1} are 0. In stage 1, both v_i and $v_{i+1} = 0$, thus the tangential velocity is given by (eq 2.7 from Snyder and Doherty[1]):

$$v_{1,i}^t = \frac{v_{i-1}}{\sin(\alpha_{i-1,i})} \tag{6}$$

In stage 2, only $v_{i+1} = 0$, and thus the tangential velocity is given by (eq 2.8 from Snyder and Doherty[1]):

$$v_{2,i}^t = \frac{-v_i \cos(\alpha_{i,i+1})}{\sin(\alpha_{i,i+1})} + \frac{v_{i-1} - v_i \cos(\alpha_{i-1,i})}{\sin(\alpha_{i-1,i})} \tag{7}$$

The tangential velocity in stage 3 is equivalent to eq 5 since no velocities are 0.

If an edge i disappears during the first rotation of a spiral, then τ_{i+1}^{rot} is still affected by edge i before edge i disappears. Once edge i has disappeared, edge i-1 becomes the adjacent edge that affects τ_{i+1}^{rot}. To account for this, we appropriately distribute the rotation time contributions by both edges i and i-1. To do this we split τ_{i+1}^{rot} into two parts, τ_a and τ_b where there exists some a and b such that:

$$l_{i+1,c} = a + b \tag{8}$$

where length a is created by the motion of edge i before it disappears, and length b is created by the motion of edge $i-1$ after edge i has disappeared. Thus,

$$\tau_{i+1}^{rot} = \tau_a + \tau_b = \frac{a}{\left(v_{1,i+1}^t\right)^*} + \frac{b}{\left(v_{1,i+1}^t\right)^\Delta} \tag{9}$$

where

$$\left(v_{1,i+1}^{t}\right)^{*} = \frac{v_i}{\sin(\alpha_{i,i+1})} \tag{10}$$

$$\left(v_{1,i+1}^{t}\right)^{\Delta} = \frac{v_{i-1}}{\sin(\alpha_{i-1,i+1})} \tag{11}$$

With these, a and b can be solved for as follows:

$$t_{dis,i} = \frac{l_{i,c}}{-v_{2,i}^{t}} = \frac{a}{\left(v_{1,i+1}^{t}\right)^{*}} = \frac{a}{\frac{v_i}{\sin(\alpha_{i,i+1})}} \tag{12}$$

where $t_{dis,i}$ is the time it takes for edge i to disappear.

$$\therefore a = \frac{l_{i,c}}{-v_{2,i}^{t}} \times \frac{v_i}{\sin(\alpha_{i,i+1})} \tag{13}$$

Then, since $a + b = l_{i+1,c}$, it follows that:

$$b = l_{i+1,c} - a \tag{14}$$

Finally once we solve for τ_{i+1}^{rot} by substituting in a and b, we find that eq 9 becomes:

$$\therefore \tau_{i+1}^{rot} = \frac{l_{i,c}}{-v_{2,i}^{t}} + \left(\frac{(l_{i+1,c} - [\frac{l_{i,c}}{-v_{2,i}^{t}}][\frac{v_i}{\sin(\alpha_{i,i+1})}])\sin(\alpha_{i-1,i+1})}{v_{i-1}}\right) \tag{15}$$

After deriving eq 15, we were interested in the calculated difference between using equations 4 and 15 when solving for the total rotation time of the spiral, τ. However, upon calculating the rotation time of multiple spirals that have disappearing edges, we found that the two equations produced exactly the same results.
Henceforth, we refer to Snyder and Doherty's use of eq 4 to solve this problem as (Method S) and our new method of using eq 15 as (Method G).

Method S discards edges that disappear such that when edges are not discarded, this means that it uses τ_{i+1}^{rot} = eq 2 when edge i does not disappear, τ_{i+1}^{rot} = eq 3 when edge i disappears.

On the other hand, we do not discard disappearing edges in Method G. When taking the sum $\sum_{i=1}^{N} \tau_{i+1}^{rot}$, we instead use τ_{i+1}^{rot} = eq 2 when edge i does not disappear, and τ_{i+1}^{rot} = eq 15 when it does.

These two methods seem quite different. However, the fact that they both give the same numerical results for all test systems suggests that the two methods are in fact identical. Therefore, we asked if it could be mathematically shown that the two methods of calculating the rotation time are equivalent. The proof that they are equivalent is given below:

Since Method S discards edge i if it disappears, the value of $\tau_{i}^{rot} + \tau_{i+1}^{rot}$ when using Method G must be equal to τ_{i+1}^{rot} in Method S(eq 3) if S and G are to be equivalent.

Start with the sum of $\tau_i^{rot} + \tau_{i+1}^{rot}$ from Method G.

$$\underbrace{\frac{l_{i,c}\sin(\alpha_{i-1,i})}{v_{i-1}}}_{\tau_i^{rot}} + \underbrace{\frac{l_{i,c}}{-v_{2,i}^t} + \left(\frac{(l_{i+1,c} - [\frac{l_{i,c}}{-v_{2,i}^t}][\frac{v_i}{\sin(\alpha_{i,i+1})}])\sin(\alpha_{i-1,i+1})}{v_{i-1}}\right)}_{\tau_{i+1}^{rot}} \tag{16}$$

$\frac{1}{v_{i-1}}$ is factored out from every term and the last term is multiplied out, giving

$$= \frac{l_{i,c}\sin(\alpha_{i-1,i}) + \left(\frac{l_{i,c}}{-v_{2,i}^t}v_{i-1}\right) + (l_{i+1,c}\sin(\alpha_{i-1,i+1}))}{v_{i-1}} + \tag{17}$$

$$\frac{-\left([\frac{l_{i,c}}{-v_{2,i}^t}][\frac{v_i}{\sin(\alpha_{i,i+1})}]\sin(\alpha_{i-1,i+1})\right)}{v_{i-1}}$$

Now, $l_{i+1,c}$ is factored out and some terms are reordered to give:

$$= \frac{l_{i+1,c}}{v_{i-1}}\Bigg[\sin(\alpha_{i-1,i+1}) + \left(\frac{l_{i,c}}{l_{i+1,c}}\right)\Bigg\{-\left(\frac{v_{i-1}}{v_{2,i}^t}\right) + \tag{18}$$

$$\left(\frac{v_i}{v_{2,i}^t}\right)\left(\frac{\sin(\alpha_{i-1,i+1})}{\sin(\alpha_{i,i+1})}\right) + \sin(\alpha_{i-1,i})\Bigg\}\Bigg]$$

It can be shown that the term within braces is equal to zero (see later). Thus, eq 18 becomes

$$= \frac{l_{i+1,c}\sin(\alpha_{i-1,i+1})}{v_{i-1}} \tag{19}$$

$$\therefore \tau_i^{rot} + \tau_{i+1}^{rot} = \frac{l_{i+1,c}\sin(\alpha_{i-1,i+1})}{v_{i-1}} \tag{20}$$

which is the same as eq 3.

Proof that the term inside braces = 0:

let θ = outer angle between edge i-1 and i = $\alpha_{i-1,i}$
let ϕ = outer angle between edge i and i+1 = $\alpha_{i,i+1}$
thus θ+ϕ = outer angle between edge i-1 and i+1 = $\alpha_{i-1,i+1}$
Substituting in θ and ϕ: $v_{2,i}^t = \frac{-v_i \cos(\phi)}{\sin(\phi)} + \frac{v_{i-1} - v_i \cos(\theta)}{\sin(\theta)}$

Starting with the original equation inside the braces:

$$-\left(\frac{v_{i-1}}{v_{2,i}^t}\right) + \left(\frac{v_i}{v_{2,i}^t}\right)\left(\frac{\sin(\alpha_{i-1,i+1})}{\sin(\alpha_{i,i+1})}\right) + \sin(\alpha_{i-1,i}) \tag{21}$$

First, substitute in θ, ϕ and θ+ϕ.

$$= -\left(\frac{v_{i-1}}{v_{2,i}^t}\right) + \left(\frac{v_i}{v_{2,i}^t}\right)\left(\frac{\sin(\theta+\phi)}{\sin(\phi)}\right) + \sin(\theta) \tag{22}$$

Then, factor out $\frac{1}{v^t_{2,i}}$ from everything.

$$= \left(\frac{1}{v^t_{2,i}}\right)\left[(-v_{i-1}) + \left(\frac{v_i\ \sin(\theta+\phi)}{\sin(\phi)}\right) + \left(v^t_{2,i}\ \sin(\theta)\right)\right] \tag{23}$$

After that, substitute in the actual value of $v^t_{2,i}$.

$$= \left(\frac{1}{v^t_{2,i}}\right)\left[-v_{i-1} + \left(\frac{v_i\ \sin(\theta+\phi)}{\sin(\phi)}\right) + \right. \tag{24}$$

$$\left.\left(\frac{-v_i\ \cos(\phi)}{\sin(\phi)} + \frac{v_{i-1} - v_i\ \cos(\theta)}{\sin(\theta)}\right)\sin(\theta)\right]$$

Distribute the $\sin(\theta)$.

$$= \left(\frac{1}{v^t_{2,i}}\right)\left[-v_{i-1} + \left(\frac{v_i\ \sin(\theta+\phi)}{\sin(\phi)}\right) + \right. \tag{25}$$

$$\left.\left(\frac{-v_i\ \cos(\phi)\sin(\theta)}{\sin(\phi)}\right) + v_{i-1} - v_i\ \cos(\theta)\right]$$

Here, the v_i's cancel each other out, and $-v_i\ \cos(\theta)$ gets multiplied by $\frac{\sin(b)}{\sin(b)}$.

$$= \left(\frac{1}{v^t_{2,i}}\right)\left[\left(\frac{v_i\ \sin(\theta+\phi)}{\sin(\phi)}\right) + \left(\frac{-v_i\cos(\phi)\sin(\theta)}{\sin(\phi)}\right) + \left(\frac{-v_i\ \cos(\theta)\sin(\phi)}{\sin(\phi)}\right)\right] \tag{26}$$

After that, combining the terms with $\sin(\phi)$ in the denominator gives

$$= \left(\frac{1}{v^t_{2,i}}\right)\left[\left(\frac{v_i\ \sin(\theta+\phi)}{\sin(\phi)}\right) + (-v_i)\left(\frac{\cos(\phi)\sin(\theta) + \ \cos(\theta)\sin(\phi)}{\sin(\phi)}\right)\right] \tag{27}$$

A trig identity simplifies the last term.

$$= \left(\frac{1}{v^t_{2,i}}\right)\left[v_i\left(\frac{\sin(\theta+\phi)}{\sin(\phi)}\right) - v_i\left(\frac{\sin(\theta+\phi)}{\sin(\phi)}\right)\right] \tag{28}$$

The two terms in square brackets cancel each other out

$$= \left(\frac{1}{v^t_{2,i}}\right)[0] \tag{29}$$

giving

$$= 0 \tag{30}$$

References

1. Snyder, R.C and M.F. Doherty, "Predicting Crystal Growth by Spiral Motion," *Proc. R. Soc A*(2009) **4b5**, 1145-71.