Phase field simulation of needle crystal growth

A.M. Mullis and P.C. Bollada

Following on from our development of a phase-field model for faceted crystal growth [1], we are now extending this to the growth of needle-like crystals. Needle like morphologies are typical of Al-based intermetallics such as $Al_{13}Fe_4$ (θ-phase, also sometimes denoted as Al_3Fe) and can produce severe detrimental effects on properties such as ductility and corrosion resistance.

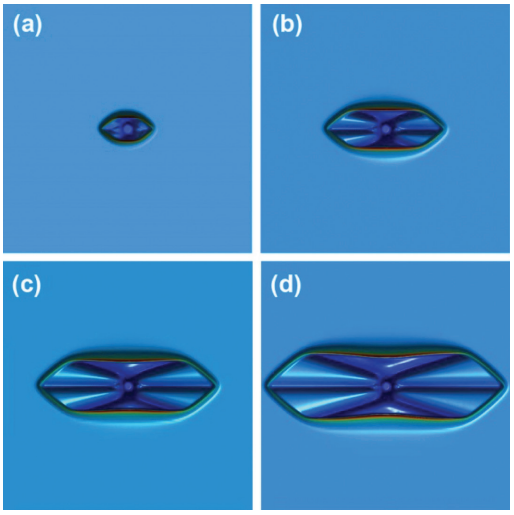

FIGURE 1. Simulated evolution of an $Al_{13}Fe_4$ needle crystal at four different times.

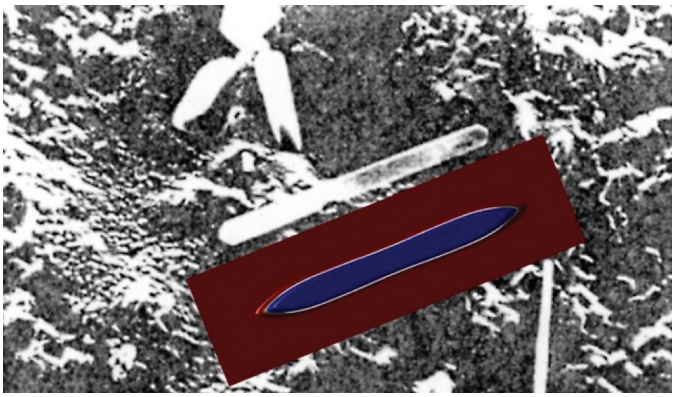

FIGURE 2. Comparison of the morphology of $Al_{13}Fe_4$ needle crystals. Experimental micrograph is for such needles growing in an Al matrix from Ref [2]. Inset is the simulation using the methodology reported here.

Therefore, understanding and controlling the formation of such morphologies is important in high value manufacturing sectors such as automotive and aerospace.

The needle morphology is in fact modelled as a modification of a faceted hexagonal crystal. For a regular hexagonal crystal with faceted sides the required anisotropy functional is:

$$\mathbf{A} = \frac{1}{2}\left\{1 + \varepsilon\sqrt{\frac{\left(\phi_x^3 - 3\phi_x\phi_y\right)^2 + q^6}{\left(\phi_x^2 + \phi_y^2 + q^2\right)^3}}\right\}\mathbf{n}$$

Here ϕ is the phase variable (1 in the solid and 0 in the liquid), ε is the anisotropy strength, $\mathbf{n}$ is the outward pointing unit normal and subscripts denote differentiation. q is a small parameter that regularizes the sharp corners permitting differentiation of the shape.

Plotting the gradient of $\mathbf{A}$, $[A_x, A_y]$ as a function of φ ($x = \cos(\varphi)$, $y = \sin(\varphi)$) gives the familiar Wulff shape for the crystal. To modify the normal hexagonal morphology to a needle we transform the function $A(x, y)$ to $A(R.x, y)$, where R is an aspect ratio in the anisotropy. However, because growth is strongly preferred along the easy directions of the anisotropy, an aspect ratio of R in the anisotropy leads to a much higher aspect ratio in the resulting crystal. This is illustrated in Figure 1, which shows four snapshots of the growth of a needle crystal. The parameters used in the simulations are $\varepsilon = 0.2$, $q = 0.1$, $R = 2$. The initial seed was a regular hexagon, wherein the initial aspect ratio is $2/\sqrt{3} = 1.15$. This increases with time to 2.33, 3.15, 3.76 and 4.37 for frames (a)-(d) respectively. In fact, we find that, to a first approximation, the length, a, grows linearly with time, t, while the width, b, grows as $\sqrt{t}$, wherein the aspect ratio increases continuously with time. In Figure 2 we make a morphological comparison between simulation and the micrograph of $Al_{13}Fe_4$ needles given in the classic review paper by Allen [2]. In both cases the aspect ratio is around 12 although currently the methodology does not correctly reproduce the angles at the crystal tip. This is being corrected by applying the aspect ratio factor R on a hexagonal basis function, rather than an orthogonal Cartesian basis.

REFERENCES:

[1] P.C. Bollada, P.K. Jimack and A.M. Mullis. Faceted and dendritic morphology change in alloy solidification. *Computational Materials Science*, 144 (2018), 76-84. DOI: 10.1016/j.commatsci.2017.12.007.

[2] C.M. Allen, K.A.Q. O'Reilly, B. Cantor and P.V. Evans. Intermetallic phase selection in 1xxx series Al alloys. *Progress in Materials Science*, 43 (1998), 89-170. DOI: 10.1016/S0079-6425(98)00003-6.