# Transient nucleus growth in liquid crystals

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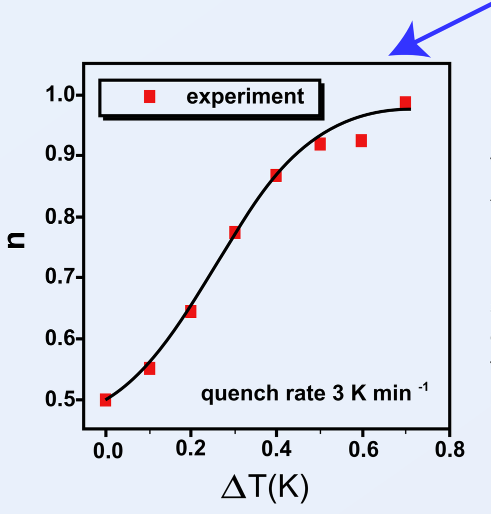
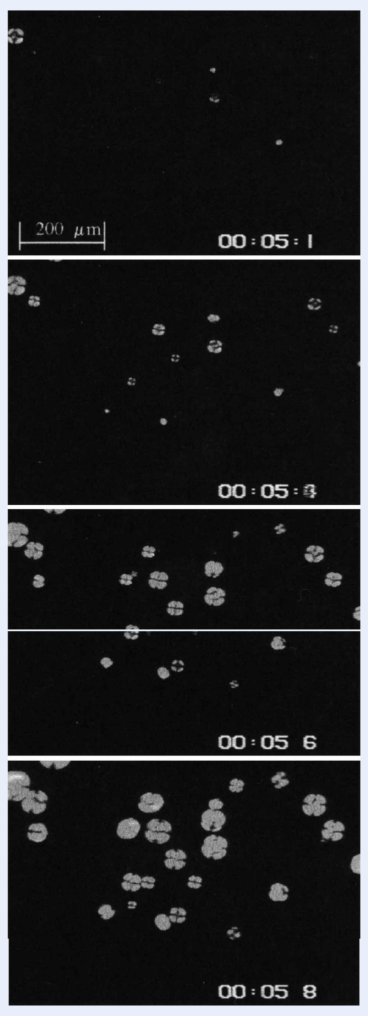
## Motivation

- In the 1st order isotropic to nematic transition of liquid crystals the radius of a nematic domain grows as $R \propto t^n$, where $n$ has been found[1,2] to depend on the undercooling $\Delta T = T - T_c$, where $T_c$ is the coexistence temperature
- The radius of a nematic domain grows as $R \propto t^{1/2}$ for low undercooling.
- The radius grows as $R \propto t^1$ for high undercooling.
- $n(\Delta T)$ resembles an S-curve as a function of $\Delta T$




**RIGHT:** Nematic germs of PCH5 growing out of the isotropic phase. In the lower right corner of each picture the time (in seconds and milliseconds) after the temperature quench is given. The undercooling ΔT is 0.15K.
Figure and caption adapted from ref. 1

**LEFT:** Experimentally determined growth exponent n as a function of undercooling ΔT. Errors are in the order of the size of the symbols. The data confirm the theoretically predicted change of n=1/2 for ΔT=0 K to n→1 for large quench depths.
Figure and caption adapted from ref. 2

## Latent heat and nucleus growth

For a first order phase transition the change of phase is accompanied by release or uptake of latent heat. The diffusion of latent heat away from the growing nucleus may explain the $R \propto t^{1/2}$ growth for low undercooling.

## Methods

Two coupled equations[3]:

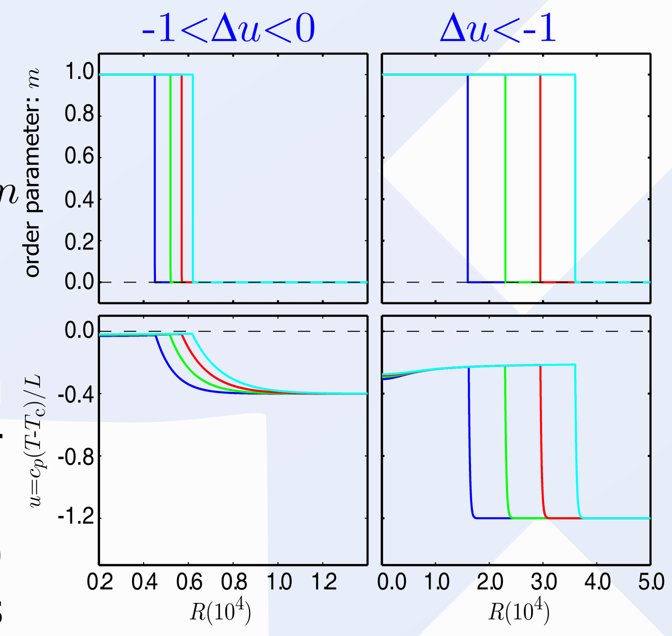
$$(1)\ \frac{\partial m}{\partial t} = \frac{1}{2}\nabla^2 m - 2m(m-1)(2m-1) + \delta u m$$

$$(2)\ \frac{\partial u}{\partial t} = \frac{1}{2p}\nabla^2 u + 2m\frac{\partial m}{\partial t}$$

$$\boxed{\begin{aligned}\delta &= \frac{\xi_m}{3\gamma}\frac{L_c}{c_p}\frac{L_c}{T_c}\frac{\rho_c}{M_W}\\ p &= \sqrt{2}\gamma\frac{M_W}{\rho_c}\frac{T_c}{L_c}\frac{\beta}{D_T}\end{aligned}}$$

(1) Time dependent Landau Ginzburg equation for the evolution of the order parameter field based on the free energy.
(2) Heat diffusion equation ($u = c_p(T - T_c)/L$) with the change in the order parameter as the latent heat source.

We solve Eq. (1) analytically[4,5]. We integrate Eq. (2) numerically in spherical coordinates, using the solution to Eq. (1).

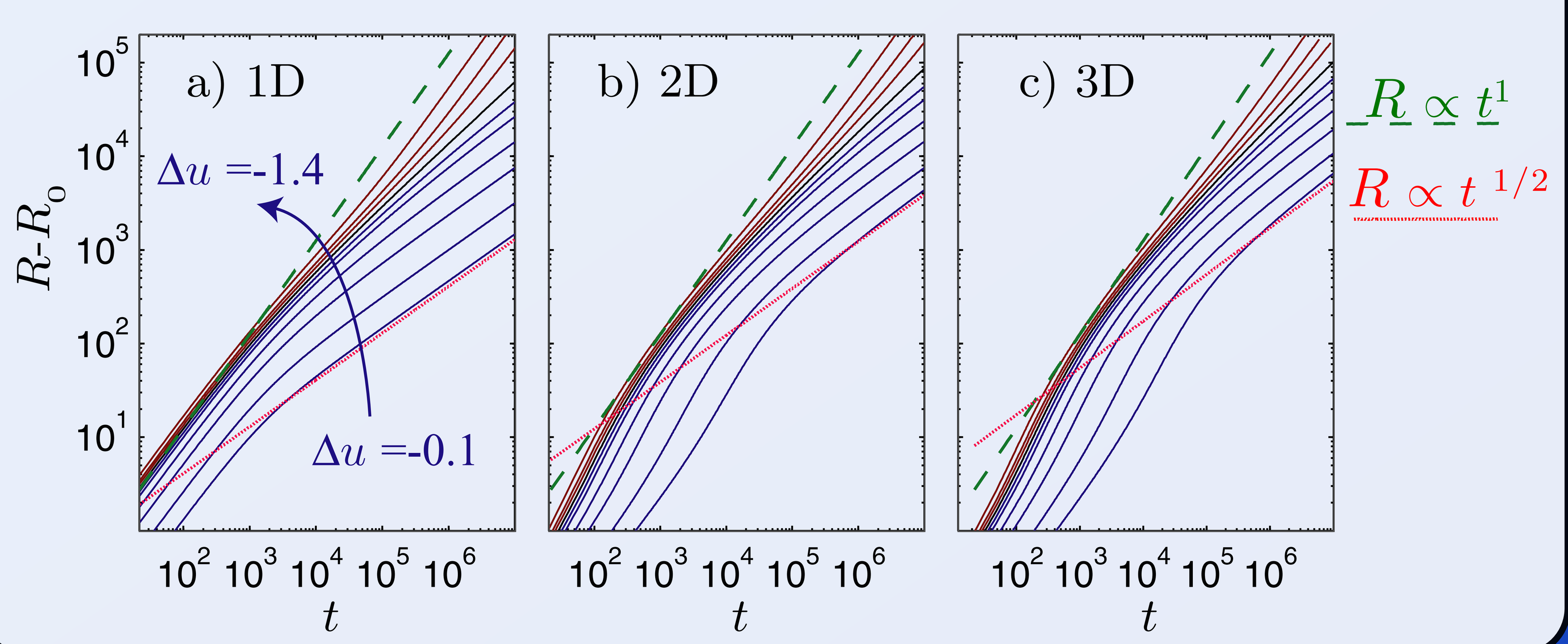



**LEFT:** For undercooling $-1<\Delta u<0$ the latent heat warms up the interface to near the coexistence temperature $u=0$. The growth is limited by thermal diffusion, and therefore $R$ will eventually grow as $R \propto t^{1/2}$.
**RIGHT:** For undercooling $\Delta u<-1$ the temperature at the front approaches a finite value $u=\Delta u+1$, and domains will grow as $R \propto t^1$.

## Radius of the growing nucleus

Here we show the radius $R(t)$ of a growing nucleus, found by integrating Eqs. (1) and (2) for different values of the undercooling temperature $\Delta u$ in 1D, 2D and 3D. Note that $R(t)$ can be described by a power law only for long times. Also note that for high undercooling the growth equals $R \propto t^1$ and for low undercoolings $R \propto t^{1/2}$.

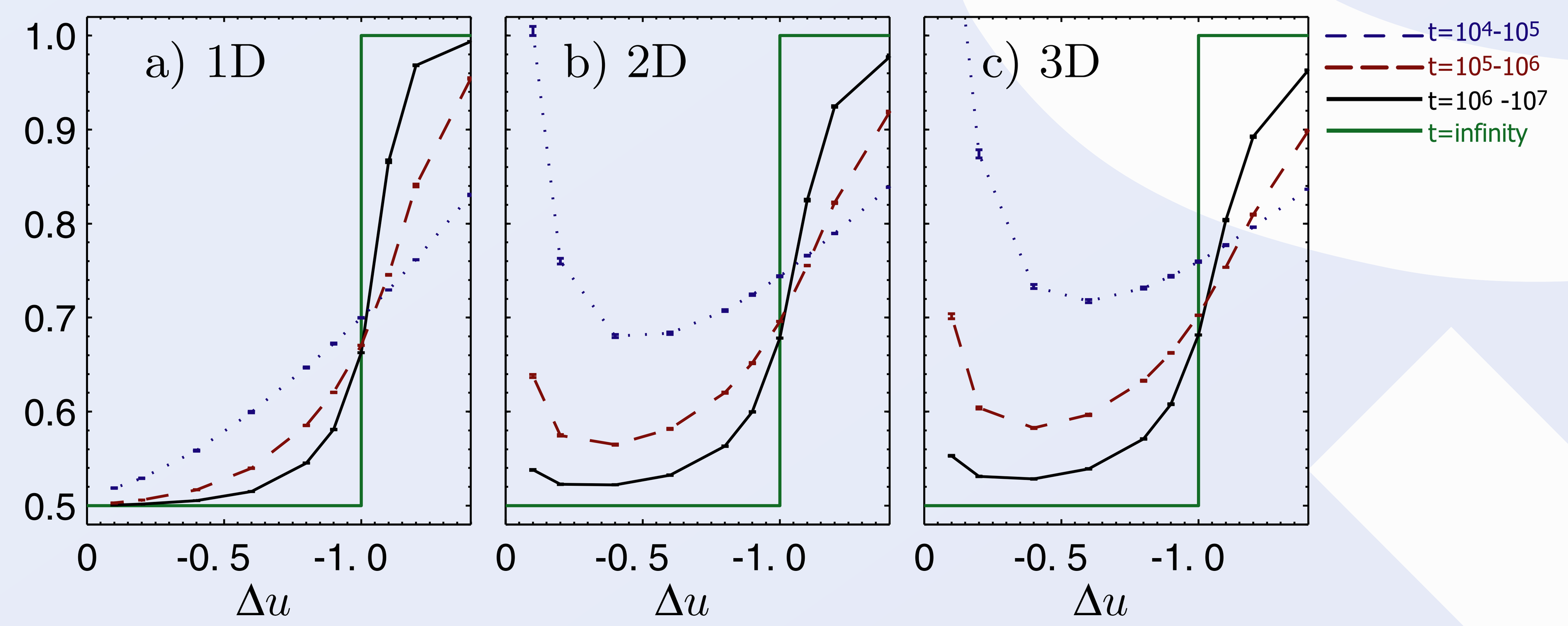
**BOTTOM:** Radius $R$-$R_o$ (in dimensionless units) of a growing nucleus in one, two and three dimensions for different values of the undercooling $\Delta u$. Parameters used: δ=0.1, p=0.033. The liquid crystal 8CB is best described by δ=1.4, p=3.4·10⁻⁶.




## Exponent of growth

- By fitting $R \propto t^n$ for different time intervals we study the time dependence of the growth exponent as a function of undercooling.
- The growth exponent follows an S-curve that sharpens with time.
- The curvature of the nucleus increases $n$ for low undercooling.
- Effect of this curvature diminishes with time as nucleus size increases.

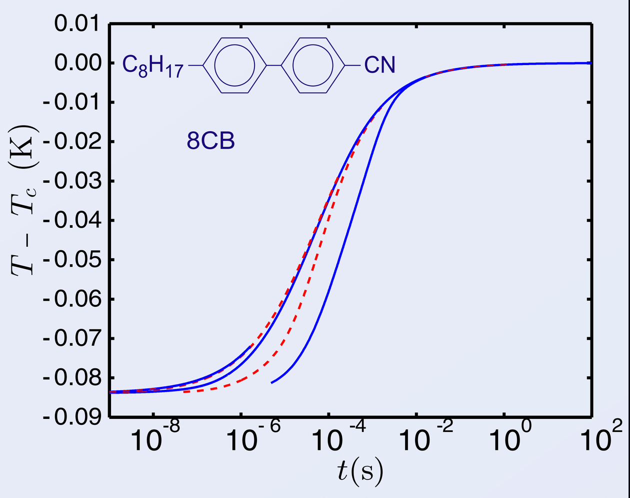
**BOTTOM:** Exponent of growth as a function of undercooling for 3 time intervals blue: $t=10^4$-$10^5$, red $t=10^5$-$10^6$, black $t=10^6$-$10^7$, green: asymptotic curve. Same data as depicted in the figure to the left of this figure.




Note that $\Delta u$=-1 equals $T = T_c - L/c_p$

## Multiple time / length scales: scaling?

- For liquid crystals the value of the parameter $p$ in Eq. (1) is very small ($10^{-6}$).
- The temperature profile is much wider than the order parameter profile. We would need in the order of $10^9$ grid points and integration over $10^{15}$ integration steps.
- In one dimension the growth velocity of the nucleus is proportional to the undercooling temperature $u(R(t))$ at the nucleus front $R(t)$ and $u(R(t))$ scales approximately with the parameter $p$ in 1D.
- By integrating Eqs. (1) and (2) for a wide range of parameters $p$ and rescaling the results, we can estimate $u(R(t))$ for extremely low values of the parameter $p$.
- Our aim is to use this scaling to determine the S-curve of the exponent of growth for parameters and length-scales suitable to describe liquid crystals.




**TOP:** Temperature at the front $u(R(t))$ estimated by rescaling simulations with different values of $p$ (from $p=10^{-6}$ to $p=0.1$) for a realistic value of δ=1.4, $\Delta u$=-0.1 in 1D. In 1D the growth velocity is approx. proportional to the undercooling.

## Applicability to liquid crystals

- The undercooling temperature $T_c - L/c_p$ separating $n$=1/2 and $n$=1 is in the range of liquid crystal (LC) nucleus growth.
- Although the latent heat is quite low in LC's, the thermal diffusivity is also very low.
- Surface tension is very low: S-curve will resemble the 1D simulation result.
- The $p$ parameter is too small for numerical integration. Using a scaling relation may help to determine the applicability more precisely.

## Conclusions

- For low undercooling $T_c > T > T_c - L/c_p$ the asymptotic behavior is $R \propto t^{1/2}$, due to the diffusion of latent heat.
- For high undercooling $T < T_c - L/c_p$ the asymptotic behavior is $R \propto t^1$.
- Because the time at which asymptotic behavior is reached depends on the undercooling, experimentally an S-curve is measured. Asymptotic behavior may never be reached because nuclei start to coalesce.

## References

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