Phase-field solidification model for pure materials

The solidification of a pure element can be described by a single non-conserved order parameter $\eta(r)$. This order parameter describes the liquid phase $(\eta = 0)$ and solid phase ($\eta = 1$). The free energy of this system $F[\eta(r)]$ as can be given as

$$F[\eta(\boldsymbol{r})] = \int \left[\omega\eta^2(1-\eta)^2 - \Delta f\ h(\eta) + \frac{\kappa}{2}(\nabla\eta)^2\right] dV$$

Where ω is the height of the double-well barrier, κ is the gradient energy coefficient, Δf is the driving force for transformation from solid to liquid and $h(\eta)$ is the interpolation function. In this example, the 5th degree polynomial $h(\eta) = \eta^3(10 - 15\eta + 6\eta^2)$ is used as interpolation function. The driving force for solidification is given by

$$\Delta f = f^l(T) - f^s(T)$$

Where $f^l(T)$ is the free energy of the liquid phase and $f^s(T)$ is the free energy of solid phase. The free energies of the individual phases were directly obtained through PanEngine/PanDataNet. The kinetic evolution of the system is performed based on Allen-Cahn equation:

$$\frac{\partial\eta}{\partial t} = -M_\eta \frac{\delta F}{\delta\eta} = M_\eta\left[\kappa\nabla^2\eta - 4\omega\eta\left(\eta - \frac{1}{2}\right)(\eta - 1) - \Delta f\frac{\partial h}{\partial\eta}\right]$$

Where M_η is the mobility of the order parameter. The model parameters κ and ω were determined by fixing the interfacial energy (γ) and interfacial width (W).

$$\gamma = \frac{\sqrt{\kappa\omega}}{3\sqrt{2}};\quad W = 2.94\sqrt{\frac{2\kappa}{\omega}}$$

The interfacial width (W) is defined as the region where the order parameter value η changes from 0.05 to 0.95. The mobility of the order parameter M_η can be determined from the physical interface mobility $\mu\ \left(\frac{m^4}{J.sec}\right)$ as $M_\eta = \mu\sqrt{\frac{\omega}{18\kappa}}$. In one-dimensional simulation, the physical interface mobility μ can realized as the ratio of interface velocity $v\left(\frac{m}{s}\right)$ and $\Delta f\left(\frac{J}{m^3}\right)$: $\mu = \frac{v}{\Delta f}$.

For the purposes of the numerical simulation, the Allen-Cahn equation is normalized as:

Table 1:List of all the model parameters

Model parameter	Non-dimensional form	Notes
$l_o(m)$	-	Grid size
$G_n\ \left(\frac{J}{mol}\right)$	-	Energy normalization factor

$B_n\left(\frac{J}{mol}\right)$	-	Mobility normalization factor
$\kappa\left(\frac{J}{m}\right)$	$\tilde{\kappa} = \frac{\kappa\, V_m}{G_n l_o^2}$	Gradient energy coefficient
$\omega\ \left(\frac{J}{m^3}\right)$	$\widetilde{\omega} = \frac{\omega V_m}{G_n}$	Barrier height
$\Delta f\left(\frac{J}{m^3}\right)$	$\widetilde{\Delta f} = \frac{\mathrm{V_m}\,\Delta f}{G_n}$	Driving force for transformation.
$M_\eta\left(\frac{m^3}{J.sec}\right)$	$\widetilde{M_\eta} = \frac{M_\eta l_o^2}{B_n V_m}$	Mobility of the order parameter