

Numerical Simulations for spiral crystal growth with impurity, interlaced spiral and variable driving force

T. Ohtsuka(Gunma Univ.)

Contents:

- With impurity: case of bunching
- Interlaced spiral
- Variable driving force by distance from a screw dislocation
 - Wisker like growth
 - Hollow core like growth

By level set method:

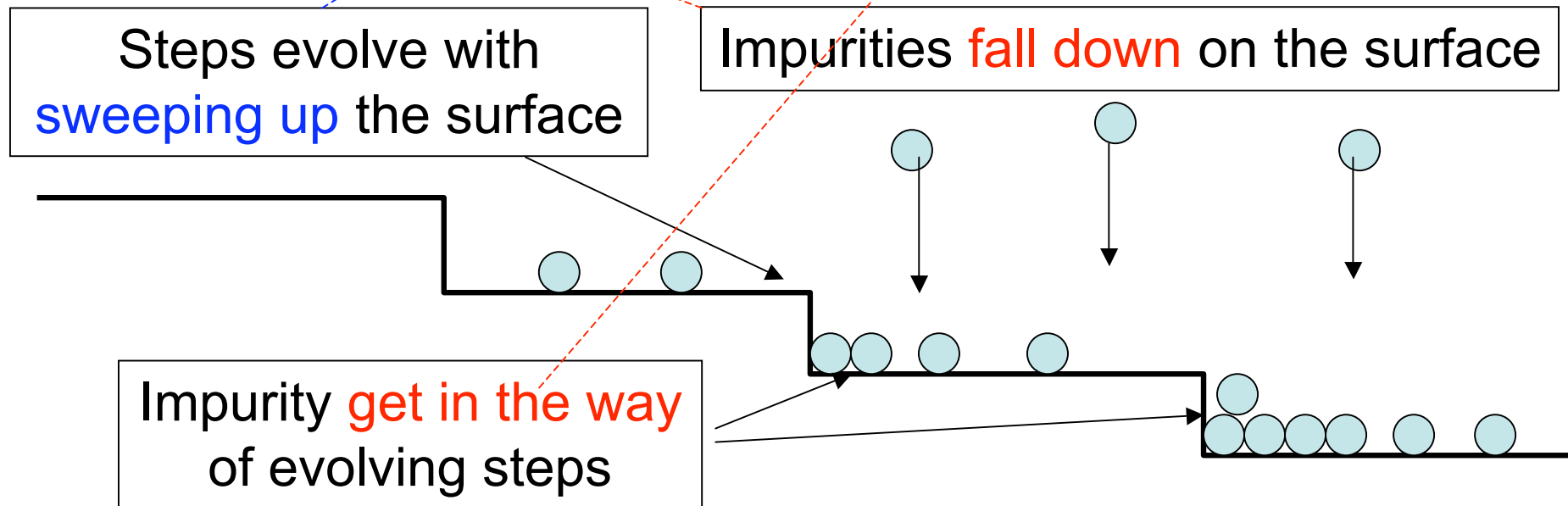
$$\Gamma_t = \bigcup_{k \in \mathbb{Z}} \{x \in \overline{W}; u(t, x) - \theta(x) = 2\pi k\}$$

✂ These models are toy models.

With impurity

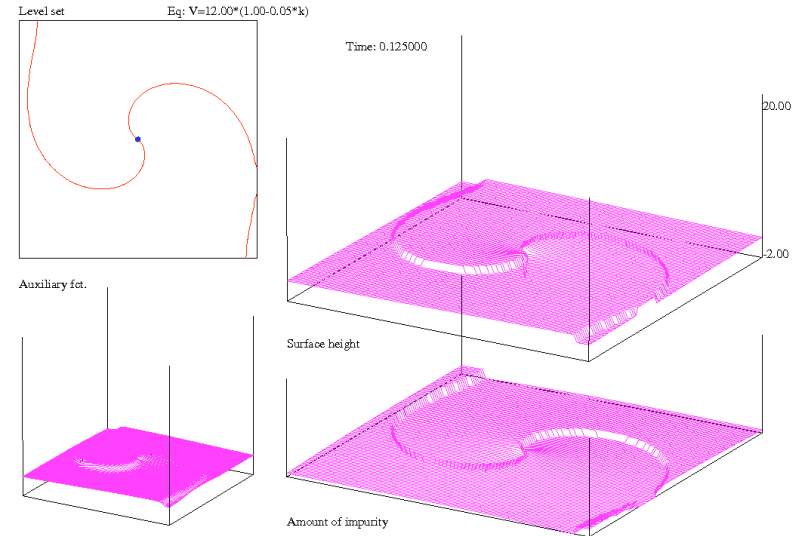
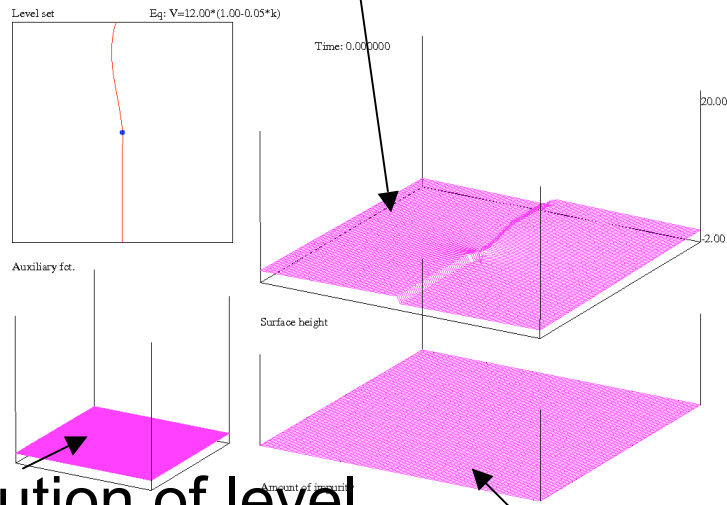
$$\left\{ \begin{array}{l} u_t - |\nabla(u - \theta)| \left\{ C(w) - \operatorname{div} \frac{\nabla(u - \theta)}{|\nabla(u - \theta)|} \right\} = 0, \\ C(w) = c_{\min} + (c_{\max} - c_{\min}) \exp(-\gamma w), \\ w_t = \mu - w \delta_{\Gamma_t}(x) \end{array} \right. \quad \text{in } (0, T) \times W$$

(Idea is due to R. Kobayashi in Allen-Cahn equation model.)



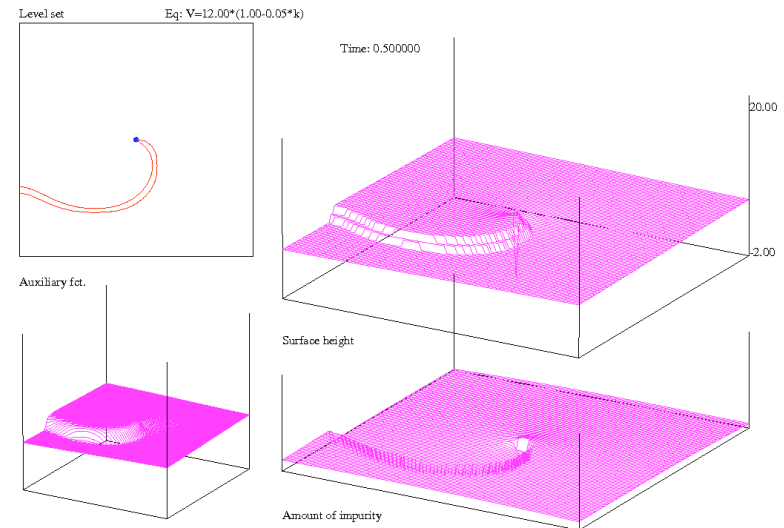
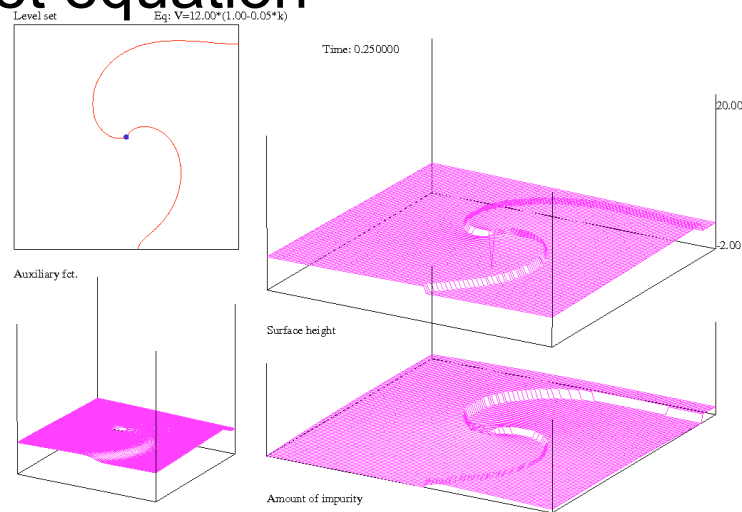
Simulation with impurity

surface



solution of level set equation

amount of impurity



Interlaced spiral

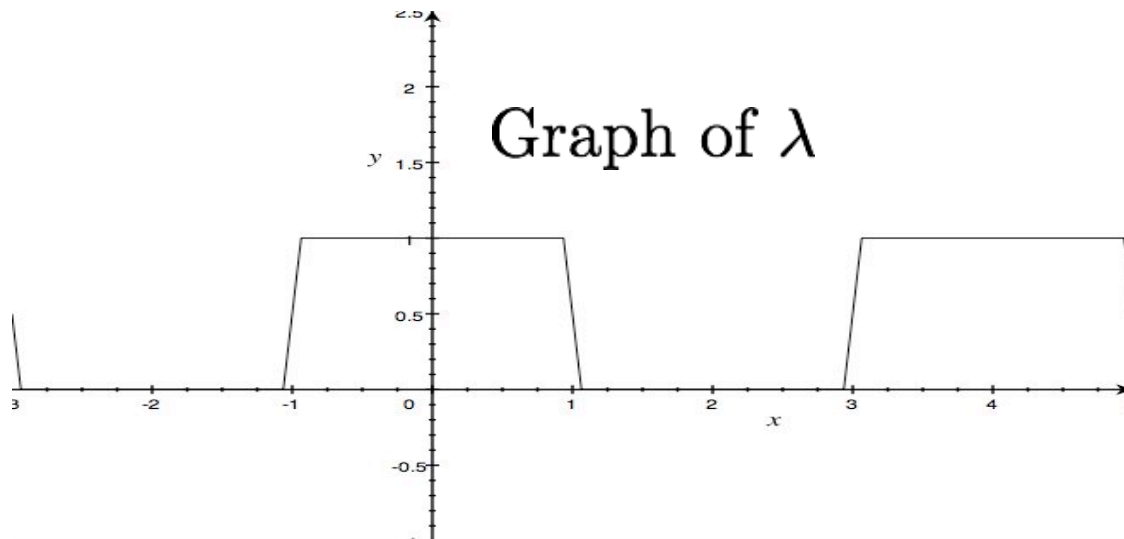
$$u_t + \lambda(u - \theta)F_1(\nabla(u - \theta), \nabla^2(u - \theta)) \\ + (1 - \lambda(u - \theta))F_2(\nabla(u - \theta), \nabla^2(u - \theta)) = 0$$

in $(0, T) \times W$

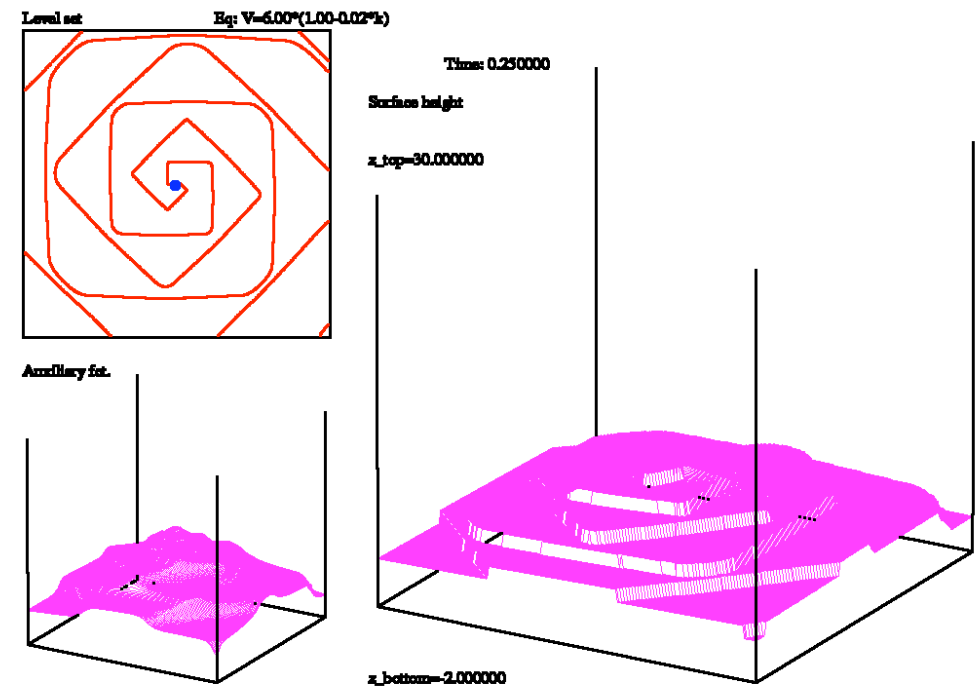
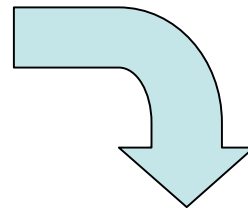
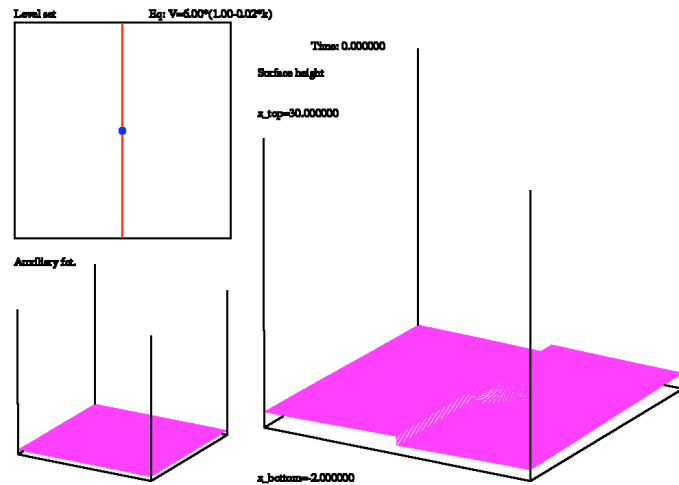
γ_i : surface energy density (anisotropy)

$$F_i(p, X) = -\gamma_i(p)(C_i + \text{tr} D^2 \gamma_i(p) X)$$

$$\lambda(u) = \{\max(-1.0, \min(-1.0, M \cos(u/2))) + 1.0\} / 2$$



Simulations of interfaced spiral



Remark:
Shape of spirals depend on λ . \Rightarrow Uniqueness of motion may be broken.

Wisker type growth

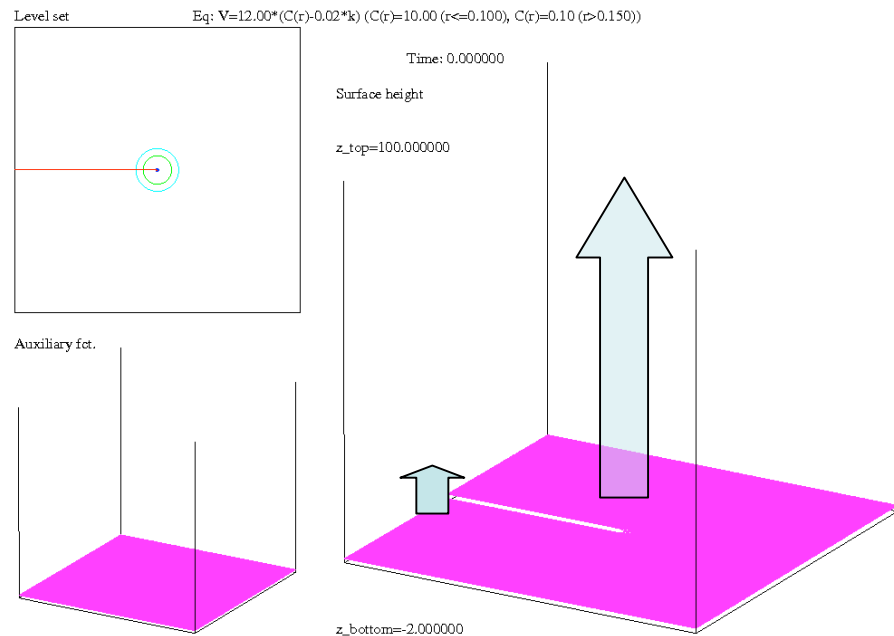
$$\begin{cases} V = C(r) - \kappa, \\ C(r) = \lambda(r)C_{int} + (1 - \lambda(r))C_{ext} \end{cases}$$

r : distance from screw dislocation,

$\lambda(r)$: cut-off function

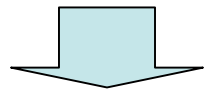
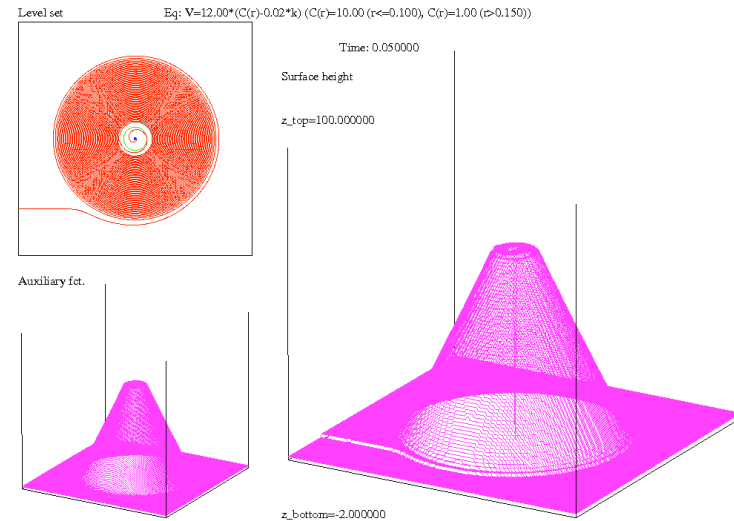
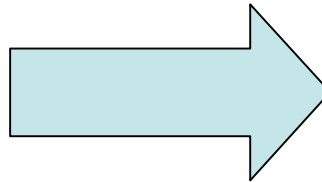
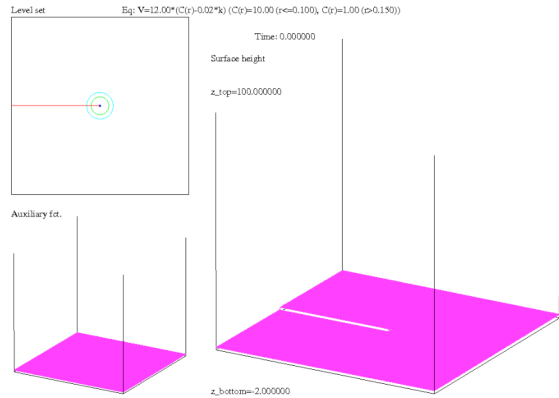
● $C_{int} > C_{ext} > 0$

A crystal around screw grows extremely around center.

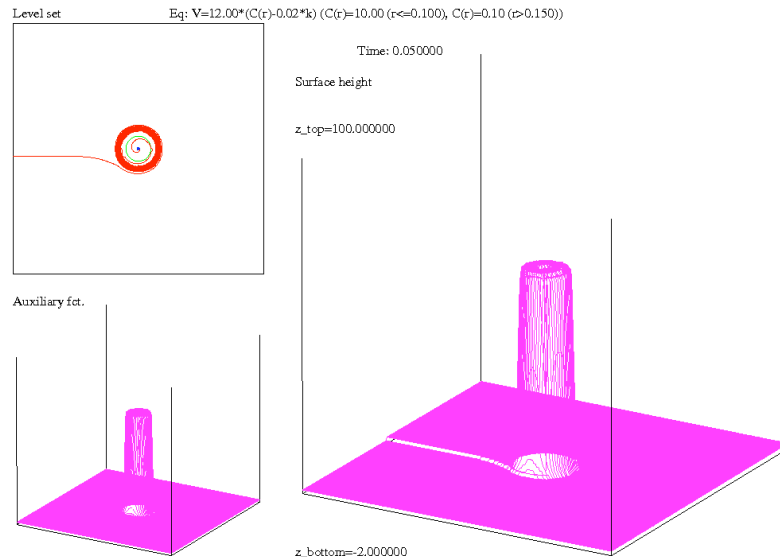


Simulation of whisker type growth

$$C_{int}=10.0, C_{ext}=1.0$$



$$C_{int}=10.0, C_{ext}=0.1$$



If whisker grows by spiral, then the crystal may need extremely high driving force around screw dislocation.

Hollow core type growth

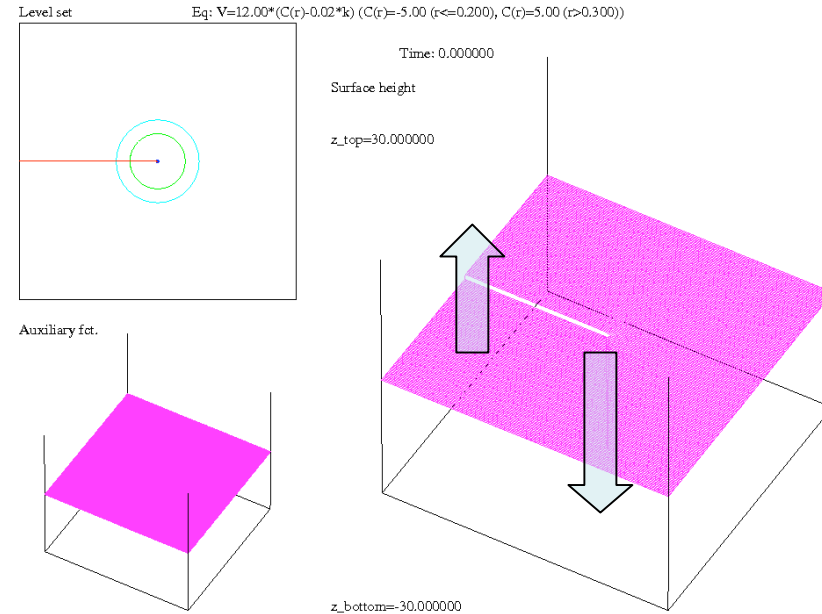
$$\begin{cases} V = C(r) - \kappa, \\ C(r) = \lambda(r)C_{int} + (1 - \lambda(r))C_{ext} \end{cases}$$

r : distance from screw dislocation,

$\lambda(r)$: cut-off function

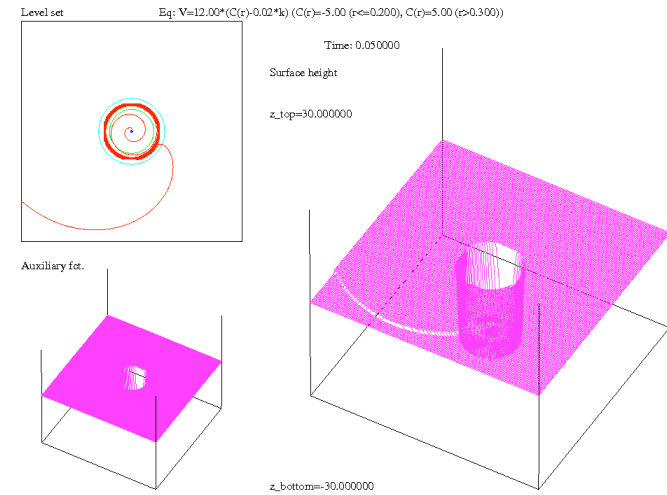
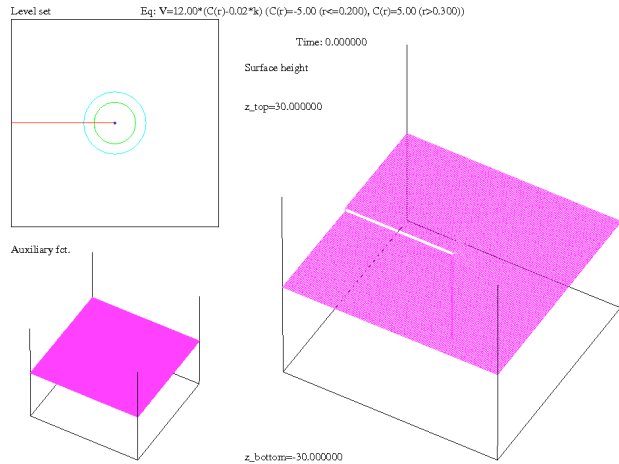
● $C_{int} < 0 < C_{ext}$

A crystal grows, but melts only around screw dislocation.

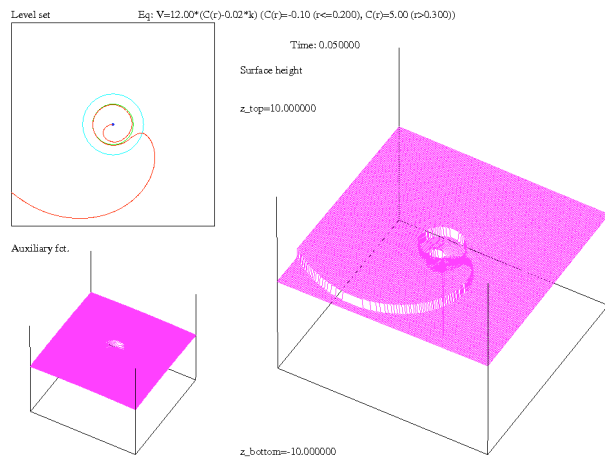


Simulations of hollow core type growth

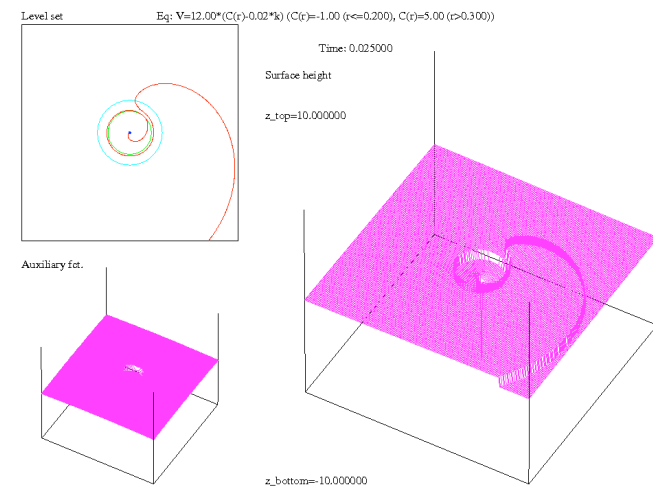
$$C_{int} = -5.0, C_{ext} = 5.0$$



$$C_{int} = -0.1, C_{ext} = 5.0$$



$$C_{int} = -1.0, C_{ext} = 5.0$$



very slow growth

melted

Concluding Remarks

- These equations are **toy models**: just suggestion of step motion by **simple equations**.
- [Impurity, interlace, hollow core] Bunching (**discontinuity**) appear in all equations. These are the crucial difficulties for mathematical analysis, even on well-posedness.
 - Interlaced spiral model is similar to the **shock waves**.
 - Wisker and hollow core type have **singular circle**.
 - With impurity model has singularities on **whole steps**.
- [Wisker] If wisker grows by screw dislocation, then the crystal has **almost zero driving force** on the far domain.
- [Hollow core] There may be two kind of cores: by melted, or by very slow growth only around screw dislocation.