Homogenization and Two–Scale Model for Liquid Phase Epitaxy

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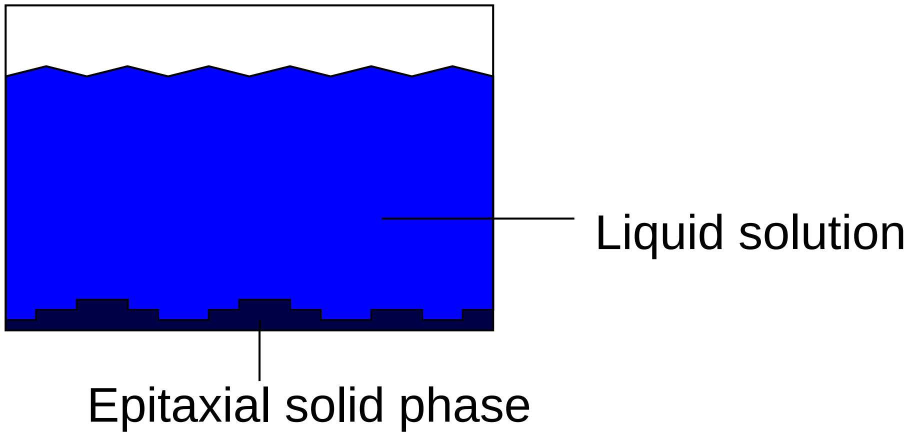
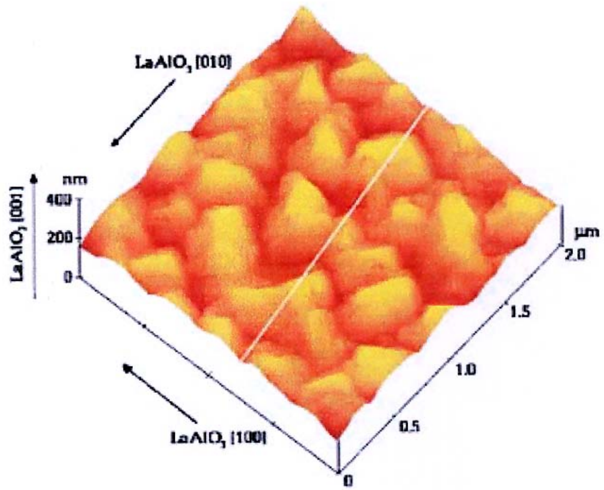
Epitaxy

Growth of thin solid layers by deposition of atoms
Application: production of semiconductors

Liquid phase epitaxy: Atoms are solved in liquid and transported to surface by diffusion and convection





Observation: Microstructures of spiral shape

Burton Cabrera Frank (BCF) model

Continuum model for epitaxy

Deposited atoms move around by surface diffusion till they incorporate into existing monoatomar layer or desorb from surface

c^S — surface density of atoms (number of atoms / area)
D_S — surface diffusivity
τ_S — mean time for desorption
τ_V — mean time for deposition

Equation for surface diffusion

$$\partial_t c^S - D_S \Delta c^S = \frac{1}{\tau_V} - \frac{c^S}{\tau_S}$$

Interface condition at boundaries of monoatomar layers

$$c^S = c_{\text{eq}}\Big(1 + \kappa\Omega\gamma/(k_B T)\Big)$$
$$v^S = D_S\Omega\left[\frac{\partial c^S}{\partial n}\right]$$

c_{eq} — equilibrium surface concentration

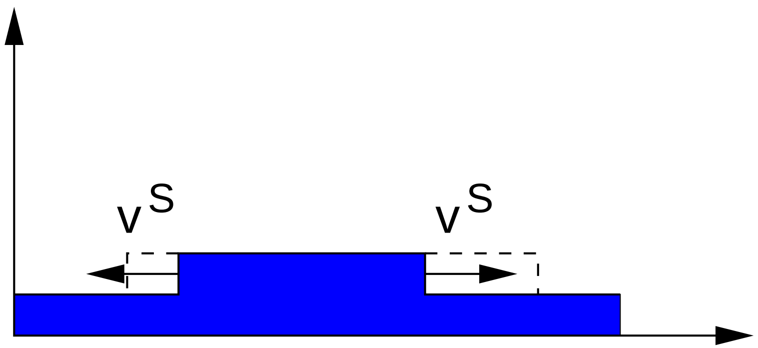
κ — curvature of steps

Ω — area of single atom

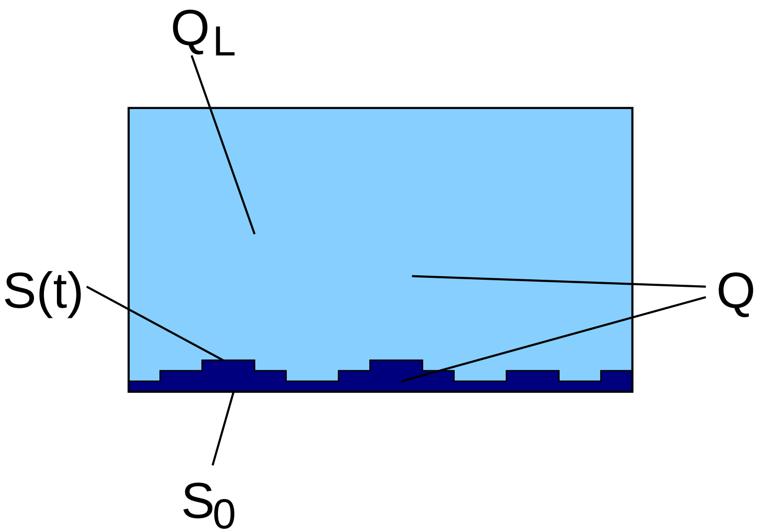
γ — step stiffness

$k_B T$ — thermal energy

$[\cdot]$ — jump of fluxes



Model for liquid phase epitaxy



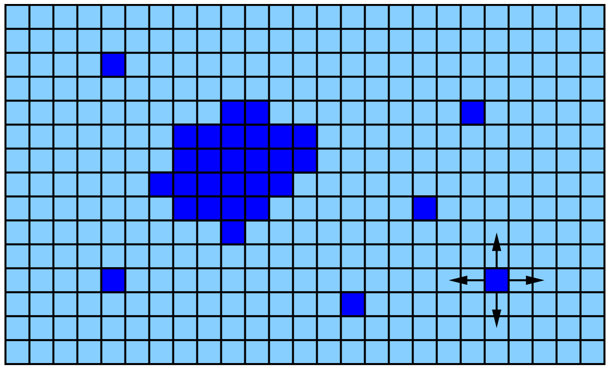
v	—	velocity
p	—	pressure
c^V	—	liquid concentration in Q
c^S	—	surface concentration on S_0
Φ	—	phase field, number of atom layers of solid

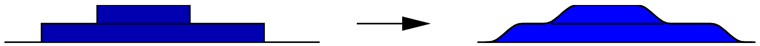
Navier–Stokes and convection–diffusion equations in $Q_L(t)$

$$\begin{aligned} \nabla \cdot v &= 0 \\ \partial_t v + (v \cdot \nabla) v - \eta \Delta v &= \nabla p \\ \partial_t c^V + v \cdot \nabla c^V - D_V \Delta c^V &= 0 \end{aligned}$$

Phase field version of Burton–Cabrera–Frank (BCF) model on S_0

$$\partial_t c^S - D_S \Delta c^S + \Omega^{-1} \partial_t \Phi = \frac{c^V}{\tau_V} - \frac{c^S}{\tau_S}$$
$$\alpha \xi^2 \partial_t \Phi - \xi^2 \Delta \Phi + f'(\Phi) + g(c^S, \Phi) = 0$$





- τ_V, τ_S — rates of deposition and desorption of atoms
- Ω — area of atom
- f — multi–well potential
- g — deviation from equilibrium concentration
- ξ — width of diffuse interface
- α — time relaxation parameter

Coupling conditions at $S(t)$, S_0

$$
\begin{aligned}
v_n &= J_S^{-1}\left(\frac{1}{\varrho_V}-\frac{1}{\varrho_E}\right)\left(\frac{m_A}{\tau_V}c^V-\frac{m_A}{\tau_S}c^S\right)\\
v_t &= 0\\
D_V\frac{\partial c^V}{\partial n} &= J_S^{-1}\left(1-c^V\right)\frac{m_A}{\varrho_V}\left(\frac{c^S}{\tau_S}-\frac{c^V}{\tau_V}\right)\\
\partial_t h &= \frac{m_A}{\varrho_E}\left(\frac{c^V}{\tau_V}-\frac{c^S}{\tau_S}\right)
\end{aligned}
$$

m_A — mass of atom

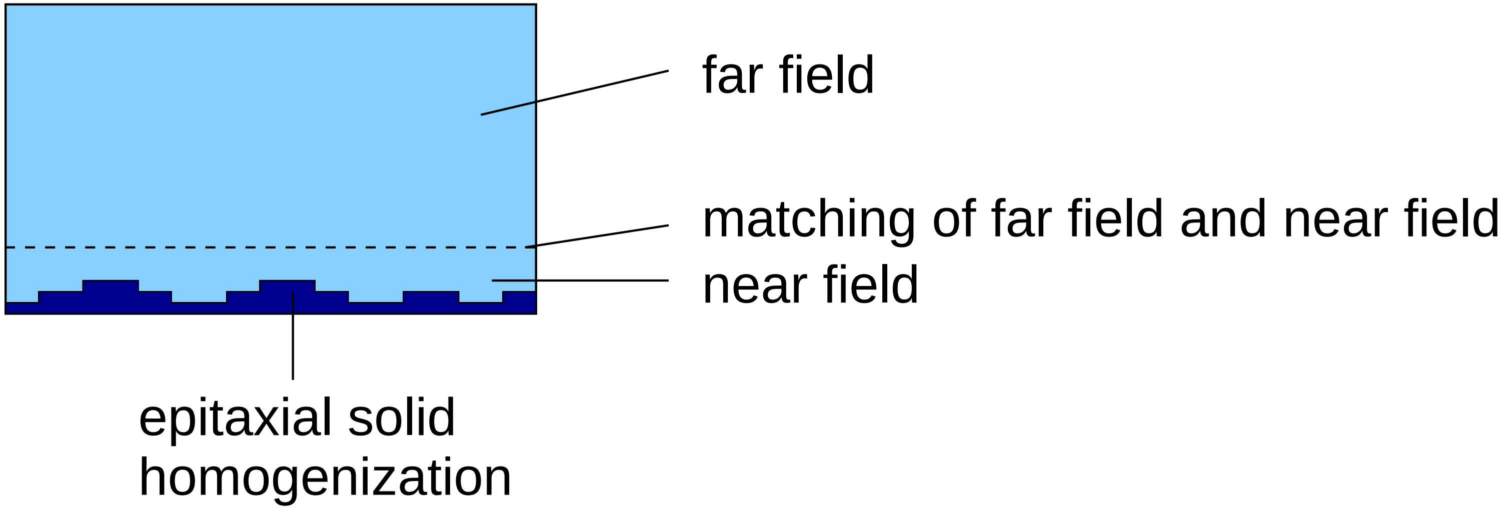
ϱ_V / ϱ_E — density in liquid / solid

h — height of epitaxial solid

J_S — density of surface measure of S, parametrized over S_0

Homogenization

Phenomena: Oscillations of scale ε on epitaxial solid layer
boundary layer close to S in liquid



Scaling of parameters:

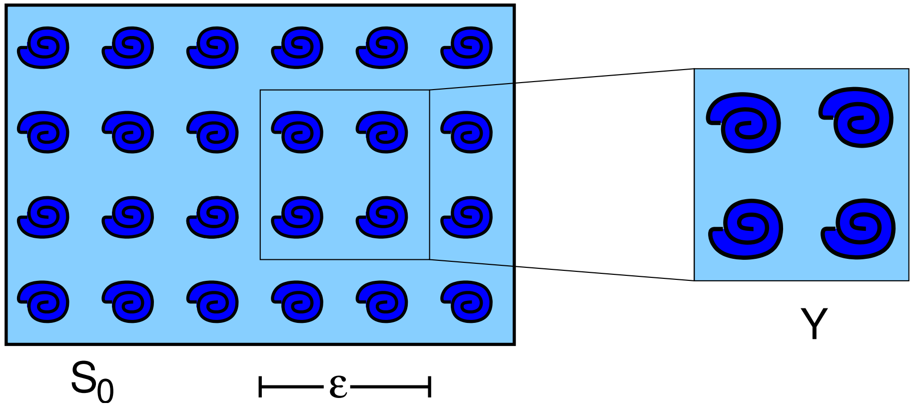
$$\Omega = \varepsilon^2 \Omega_0,\ m_A = \varepsilon^3 m_A^0,\ \tau_V = \varepsilon^3 \tau_V^0,\ D_S = \varepsilon^2 D_S^0,\ \xi = \varepsilon \xi_0,\ \alpha = \varepsilon^{-2} \alpha_0$$

Homogenization by asymptotic expansion on epitaxial surface

$$c_\varepsilon^S(t,x) = \varepsilon^{-2} c_0^S(t,x,x/\varepsilon) + \varepsilon^{-1} c_1^S(t,x,x/\varepsilon) + \cdots$$

$$\Phi_\varepsilon(t,x) = \Phi_0(t,x,x/\varepsilon) + \varepsilon \Phi_1(t,x,x/\varepsilon) + \cdots$$

$c_\ell^S, \Phi_\ell : I \times S_0 \times Y \to \mathbb{R}$, $Y \subset \mathbb{R}^2$ unit cell / periodicity cell



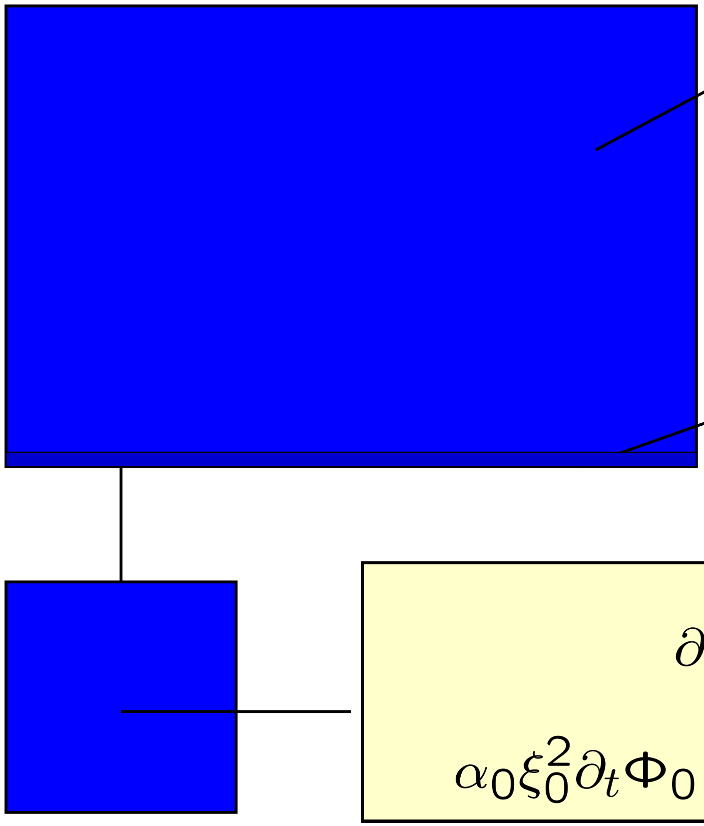
Matched asymptotic expansion in liquid

$$c_\varepsilon^V(t,x) = \varepsilon c_0^V(t,x,x/\varepsilon) + \varepsilon^2 c_1^V(t,x,x/\varepsilon) + \cdots$$

$$v_\varepsilon(t,x) = v_0(t,x,x/\varepsilon) + \varepsilon v_1(t,x,x/\varepsilon) + \cdots$$

$$p_\varepsilon(t,x) = p_0(t,x,x/\varepsilon) + \varepsilon p_1(t,x,x/\varepsilon) + \cdots$$

Homogenized model



$$\partial_t c_0^V + (v_0 \cdot \nabla) c_0^V - D_V \Delta c_0^V = 0$$

$$\partial_t v_0 + (v_0 \cdot \nabla) v_0 - \eta \Delta v_0 = \nabla p_0$$

$$\nabla \cdot v_0 = 0$$

$$D_V \frac{\partial c_0^V}{\partial n} = \frac{m_A^0}{\varrho_V} \left(\frac{\overline{c}_0^S}{\tau_S} - \frac{c_0^V}{\tau_V^0} \right)$$

$$\partial_t c_0^S - D_S^0 \Delta_y c_0^S + \Omega_0^{-1} \partial_t \Phi_0 = \frac{c_0^V}{\tau_V^0} - \frac{c_0^S}{\tau_S}$$

$$\alpha_0 \xi_0^2 \partial_t \Phi_0 - \xi_0^2 \Delta_y \Phi_0 + f'(\Phi_0) + g(c_0^S, \Phi_0) = 0$$

$$\overline{c}_0^S(t,x) = \textstyle\int_Y c_0(t,x,y)\, dy$$

Analysis of macroscopic problem

Navier–Stokes system decouples $\Rightarrow$ treat v_0 as given velocity

$$\partial_t c_0^V + (v_0 \cdot \nabla) c_0^V - D_V \Delta_y c_0^V = 0 \quad \text{in } Q$$
$$D_V \frac{\partial c_0^V}{\partial n} = \frac{m_A^0}{\varrho_V} \left(\frac{\overline{c}_0^S}{\tau_S} - \frac{c_0^V}{\tau_V^0} \right) \quad \text{on } S_0$$

Existence and uniqueness of solution

A priori estimates

$$\left\| c_0^V \right\|_{L_2(0,t_0;H^1(Q))} \leq C_1 + C_2 t_0^{1/r} \left\| \overline{c}_0^S \right\|_{L_2(I \times S_0)}, \qquad r > 0$$
$$\left\| c_0^V \right\|_{H^\beta(I;L_2(Q))} \leq C_3 + C_4 \left\| \overline{c}_0^S \right\|_{L_2(I \times S_0)}, \qquad \beta > 0$$

Continuity estimate

$$\left\| c_0^{V1} - c_0^{V2} \right\|_{L_2(I;H^1(Q))} \leq C_1 \left\| \overline{c}_0^{S1} - \overline{c}_0^{S2} \right\|_{L_2(I \times S_0)}$$

Analysis of microscopic problem

$$\begin{aligned} \partial_t c_0^S - D_S^0 \Delta_y c_0^S &= \frac{1}{\tau_V^0} c_0^V - \frac{1}{\tau_S} c_0^S \\ \alpha_0 \xi_0^2 \partial_t \Phi_0 - \xi_0^2 \Delta_y \Phi_0 + f'(\Phi_0) + g(c_0^S, \Phi_0) &= 0 \end{aligned}$$

Existence and uniqueness of solution for fixed $x \in S_0$

A–priori estimate

$$\left\| c_0^S \right\|_{L_2(I;H^1(Y))} + \|\Phi_0\|_{H^1(I\times Y)} \leq C_1 + C_2 \left\| c_0^V \right\|_{L_2(I)}$$

Continuity estimate

$$\left\| \Phi_0^1 - \Phi_0^2 \right\|_{H^1(I\times Y)} + \left\| c_0^{S1} - c_0^{S2} \right\|_{L_2(I;H^1(Y))} \leq C_1 \left\| c_0^{V1} - c_0^{V2} \right\|_{L_2(I)}$$

Analysis of coupled problem

Schauder fixed point theorem applied to

$$\mathscr{S} = \underbrace{\mathscr{S}_1}_{c_0^V \to (c_0^S, \Phi_0^S)} \circ \underbrace{\mathscr{S}_2}_{\overline{c}_0^S \to c_0^V} : \mathscr{X} \to \mathscr{X}, \; \mathscr{X} = L_2(0, t_0; H^\gamma(Q)), \; \frac{1}{2} < \gamma < 1$$

Combination of a priori estimates

$$\left\| \mathscr{S}\left(c_0^V\right) \right\|_{L_2(0,t_0;H^1(Q))} \leq C_1 + C_2 t_0^{1/r} \left\| c_0^V \right\|_{L_2(0,t_0;H^\gamma(Q))}$$
$$\left\| c_0^V \right\|_{H^\beta(I;L_2(Q))} \leq C_3 + C_4 \left\| \overline{c}_0^S \right\|_{L_2(I \times S_0)}$$

$\Rightarrow$ existence of solution for sufficiently small t_0

t_0 independent of initial data $\Rightarrow$ existence of solution for arbitrary t_0

Uniqueness of solution by combination of continuity estimates

Justification of homogenization limit

Solution of original model of scale ε:

$$\left(v_\varepsilon, p_\varepsilon, c_\varepsilon^V\right) : Z_\varepsilon \to \mathbb{R}^5, \qquad Z_\varepsilon = \left\{(t,x) \,|\, t \in I,\ x \in Q_\varepsilon(t)\right\}$$

$$\left(c_\varepsilon^S, \Phi_\varepsilon\right) : I \times S_0 \to \mathbb{R}^2$$

Rescaling: $\tilde{c}_\varepsilon^V = \varepsilon^{-1} c_\varepsilon^V$, $\tilde{c}_\varepsilon^S = \varepsilon^2 c_\varepsilon^S$

Solution of two–scale model:

$$\left(v_0, p_0, c_0^V\right) : I \times Q \to \mathbb{R}^5, \quad \left(c_0^S, \Phi_0\right) : I \times S_0 \times Y \to \mathbb{R}^2$$

Macroscopic reconstructions:

$$c_0^{S\varepsilon}(t,x) = c_0^S(t,x,x/\varepsilon), \quad \Phi_0^\varepsilon(t,x) = \Phi_0(t,x,x/\varepsilon)$$

Assumption: Uniform (in ε) bounds for

c_0^S, Φ_0	in $L_\infty(I \times S_0, W^2_\infty(Y)) \cap L_\infty(I; W^1_\infty(S_0; W^1_\infty(Y)))$
c_0^V	in $L_2(I; W^2_3(Q)) \cap L_2(I; W^1_\infty(Q))$
v_0	in $L_\infty(I; W^1_\infty(Q))$
$\tilde{c}_\varepsilon^V, \tilde{c}_\varepsilon^S$	in $C(I \times S_0)$
$\varepsilon\tilde{c}_\varepsilon^V, \varepsilon\tilde{c}_\varepsilon^S$	in $C(I; C^1(S_0))$

Estimate of $v_\varepsilon - v_0$, $\tilde{c}_\varepsilon^V - c_0^V$ on Z_ε:

$$\left\|\left(\tilde{c}_\varepsilon^V - c_0^V\right)(t_0)\right\|^2_{L_2(Q_\varepsilon(t_0))} + \|(v_\varepsilon - v_0)(t_0)\|^2_{L_2(Q_\varepsilon(t_0))}$$
$$\leq C_1 \int_0^{t_0} \left(\|v_\varepsilon - v_0\|^2_{L_2(Q_\varepsilon(t))} + \left\|\tilde{c}_\varepsilon^V - c_0^V\right\|^2_{L_2(Q_\varepsilon(t))}\right) dt$$
$$+ C_2\left\|\tilde{c}_\varepsilon^S - c_0^{S\varepsilon}\right\|^2_{L_2(I_{t_0} \times S_0)} + C_3\varepsilon$$

Estimate for $\widetilde{c}_\varepsilon^S - c_0^{S\varepsilon}$, $\Phi_\varepsilon - \Phi_0^\varepsilon$:

$$\left\|\left(\widetilde{c}_\varepsilon^S - c_0^{S\varepsilon}\right)(t_0)\right\|_{L_2(S_0)}^2 + \left\|\partial_t\left(\Phi_\varepsilon - \Phi_0^\varepsilon\right)\right\|_{L_2((0,t_0)\times S_0)}^2$$
$$\le C_1\left(\left\|\widetilde{c}_\varepsilon^V - c_0^V\right\|_{L_2((0,t_0)\times S_0)}^2 + \left\|\widetilde{c}_\varepsilon^S - c_0^{S\varepsilon}\right\|_{L_2((0,t_0)\times S_0)}^2 + \left\|\Phi_\varepsilon - \Phi_0^\varepsilon\right\|_{L_2((0,t_0)\times S_0)}^2\right) + C_2\varepsilon$$

Combination

$$\left\|\widetilde{c}_\varepsilon^S - c_0^{S\varepsilon}\right\|_{L_\infty(I;L_2(S_0))} + \left\|\Phi_\varepsilon - \Phi_0^\varepsilon\right\|_{H^1(I;L_2(S_0))} + \sup_{t\in I}\left(\left\|\left(\widetilde{c}_\varepsilon^V - c_0^V\right)(t)\right\|_{L_2(Q_\varepsilon(t))} + \|(v_\varepsilon - v_0)(t)\|_{L_2(Q_\varepsilon(t))}\right) \le C\varepsilon^{1/2}$$