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Analytical and Numerical Investigation of the Segregation Problem

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We consider the segregation of particles at material interfaces as it is observed during the implantation of dopants during semiconductor device fabrication. First, the resulting system of partial differential equations is analysed from the analytic point of view. After that numerical simulations, which are complicated due to possible discontinuities at the interface boundary, are carried out.

Consider two bounded domains Ω_1 and Ω_2 with particle concentrations u_1 and u_2 respectively. In the interior of each domain the diffusion equation with diffusion parameters $\alpha_i > 0$ is assumed to hold:

$$\frac{\partial u_i}{\partial t} = -\nabla \mathbf{q}_i \quad \text{in } \Omega_i \ , \quad \text{with} \quad \mathbf{q}_i = -\alpha_i \nabla u_i, \quad i = 1, 2. \tag{1}$$

The total flux density in outer normal direction $\mathbf{n}_i$ relative to Ω_i at the common interface $\Gamma_{12} = \partial\Omega_1 \cap \partial\Omega_2$ is according to Lau et. al. [1] given by

$$\mathbf{J} = \mathbf{q}_1 \cdot \mathbf{n}_1 = -\mathbf{q}_2 \cdot \mathbf{n}_2 = \beta(u_1 - \gamma u_2) \ , \tag{2}$$

where $\beta > 0$ is the transport coefficient and $\gamma > 0$ is the segregation parameter. Assuming homogeneous Neumann boundary conditions at the outer boundaries $\partial\Omega_1 \setminus \Gamma_{12}$, $\partial\Omega_2 \setminus \Gamma_{12}$, the weak formulation of the above equations is to find a solution (u_1, u_2) that fulfils the weak form

$$\begin{aligned} \int_{\Omega_1} \frac{\partial u_1}{\partial t} v_1 + \alpha_1 \nabla u_1 \nabla v_1 \ \mathrm{d}x + \beta \int_{\Gamma} (u_1 - \gamma u_2) v_1 \ \mathrm{d}A = 0 \ , \\ \int_{\Omega_2} \frac{\partial u_2}{\partial t} v_2 + \alpha_2 \nabla u_2 \nabla v_2 \ \mathrm{d}x - \beta \int_{\Gamma} (u_1 - \gamma u_2) v_2 \ \mathrm{d}A = 0 \ , \end{aligned} \tag{3}$$

for all test functions (v_1, v_2) from a suitable test space. We show that there exists a unique solution $u = (u_1, u_2) \in L^2([0,T], V) \cap H^1([0,T], V^*)$ of (3) for $u(0) = u_0 \in V$, where $V := H^1(\Omega_1) \times H^1(\Omega_2)$ and $V^* = H^{-1}(\Omega_1) \times H^{-1}(\Omega_2)$.

A numerical approximation to the solution of the segregation model (3) has been implemented into a newly developed generic finite element programming environment in C++, which allows the direct specification of the weak formulation into code. In particular, the end-user implementation of the transport terms in (3) takes the mnemonic form

```
assemble < FEMConfig >(segment1, system_matrix, rhs,
    integral< Omega >(gradient_u * gradient_v)
  + integral< Gamma<1> >( u * v )
  - integral< Interface<1> > ( u * v ) = _0_ ) ;
assemble < FEMConfig >(segment2, system_matrix, rhs,
    integral< Omega >(gradient_u * gradient_v)
  - integral< Interface<1> > ( u * v )
  + integral< Gamma<1> >( u * v ) = _0_ ) ;
```

The difficulty from the implementation point of view is the discontinuity at the transition from u_1 in Ω_1 to u_2 in Ω_2 at the common boundary Γ_{12}, because there one has to test the traces of trial functions defined in Ω_1 with traces of test functions defined on both Ω_1 and Ω_2 and vice versa. This is further complicated by the fact that interface elements can have different orientations, which especially complicates the assembly for higher order trial and test functions. We have solved these difficulties by the use of a reordering scheme based on the vertices of the interface elements.

Simulations have been carried out for a fictitious diffusive hourglass (cf. Fig. 1) with essentially the same code basis in one, two and three dimensions using a backward Euler time discretisation. Different ansatz spaces of functions with globally fixed piecewise polynomial degrees are compared.

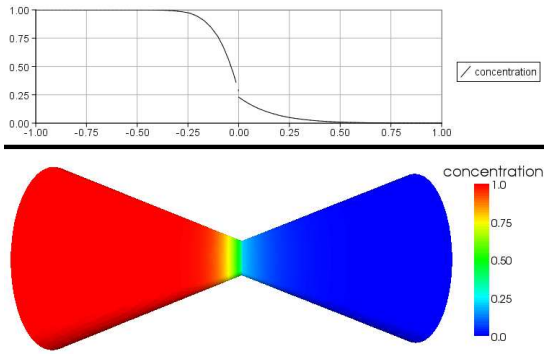

Figure 1. Particle concentration in a diffusive hourglass. The connection in the centre obeys the segregation model.

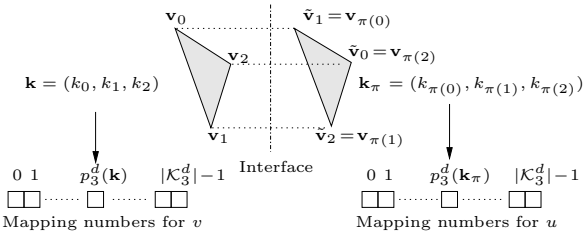

Figure 2. Automatic detection of elements with different orientation at interfaces.

References

[1] F. Lau, L. Mader, C. Mazure, Ch. Werner, M. Orlowski, *A Model for Phosphorus Segregation at the Silicon-Silicon Dioxide Interface*, in: *Applied Physics A: Materials Science & Processing*, vol. 49, p.671-675 (1989).