

AMIGOS: Analytical Model Interface & General Object-Oriented Solver

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To accurately simulate modern semiconductor process steps, a simulation tool must include a variety of physical models and numerical methods. Increasingly complex physical formulations are required to account for effects that were not important in previous generations of technology. As a specific example, the oxidation coupled with impurity diffusion mechanisms as well as chemical reactions are not well understood, and thus flexibility in definition of models is highly desirable. An object oriented approach has been applied to implementing a 1-2-3D PDE solver, which uses an analytical input interface in the manner of Mathematica, Mathcad, Matlab, etc. but is highly optimized for high performance semiconductor modeling.

1. Introduction

The development of new complex physical models and its practical realization requires a large expenditure of time. To reduce this amount of developing time we analyzed the requirements for a general solver carefully and separated the common features such as modeling for physical definitions, parameter and model library, grid-adaptation, numerical solver, simple front-end controller as well as geometry and boundary definition. As a result we developed AMIGOS that translates a mathematical formulation of any discretized coupled partial differential equation system into a highly optimized model, which will then be passed to a nonlinear numerical solver that can handle different physical models on various grids as well as interfaces and boundaries.

AMIGOS also provides several layers of access to the variety of users. For example, a process engineer (user-mode) may need only to select a model appropriate for the process step to calculate (e.g. diffusion coupled oxidation), modify the process parameters (e.g. duration, temperature, material characteristics, etc.) and defines the geometries and boundaries the process should be calculated on. On the other hand, at a lower level (developer-mode) a model developer may need to modify existing equations by adding several parameters, mathematical terms or equations, or even develop a completely new model. In contrast with previous generation of software none of the described modes needs access to and modification of the source code. In developer mode the user may choose between a one-pass or two-pass concept. The one-pass concept requires no recompilation and supports fast testing possibilities of the developed model. After finishing the test and calibrating phase the user may switch to the two-pass concept where all his modifications are translated to C code and are linked to a model library for high performance calculations on large simulation domains.

2. Design of AMIGOS

In difference to similar algorithms working with the so called ‘operator on demand’ concept [1], AMIGOS is completely independent of the kind of discretization since the model developer himself can formulate a discretization of his choice (e.g. Bernoulli discretization which is very important for semiconductor device simulation). There are no restrictions whether using scalar, field or even tensor quantities within a model and, if desired, any derived field quantity can be calculated, too. Furthermore, the user can influence the numerical behavior of the differential equation system, since he has complete control of the residual vector and its derivative (e.g. punishing terms, damping terms, etc.). Even interpolation and grid-adaptation formulations can be used within a developed model and can thus be very well fitted to the special problem. To illustrate the powerful possibilities of AMIGOS we will introduce a rigorous model of the moving grid problem arising from thermal oxidation within a semiconductor process step in the example below.

The object-oriented extension provides an efficient and versatile means to represent the organization of AMIGOS in an easy to grasp manner regarding to its complexity.

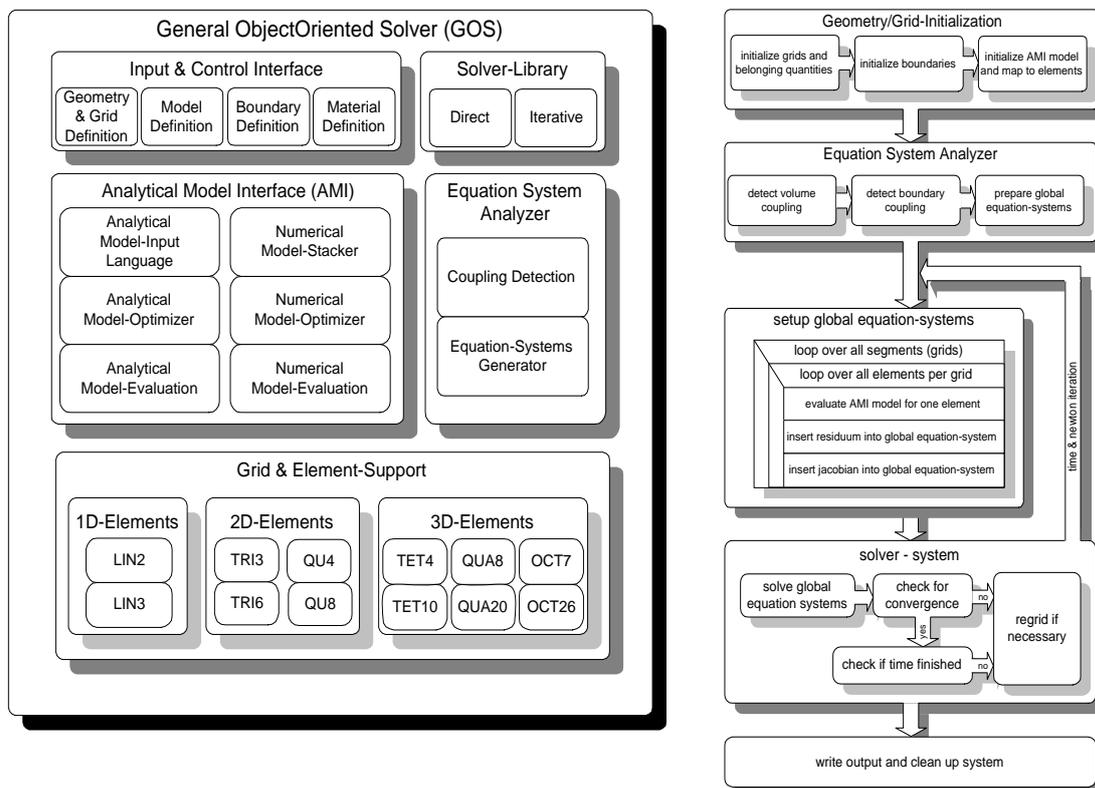


Fig. 1: Structural design and flow chart of AMIGOS

3. Example: A rigorous oxidation model

The evolution of isolation techniques and the progressive miniaturization in semiconductor devices makes it necessary to develop new and much more complex models to exactly describe the behavior of the thermal oxidation processes.

The profusion of different requirements such as chemical reactions and its resulting volume expansion as well as the mechanical stress and pressure calculations leading from elastic over viscoelastic to viscous behavior coupled with the oxidation diffusion and its recombination with Silicon represents just the modeling problem of the calculation process. In addition to these problems comes the effect that the order of magnitude varies between a few nanometers to a hundreds of nanometers which is impossible to solve without accurate grid-adaptation.

Using AMIGOS we were able to develop a model which takes all these effects into account solving a coupled differential equation system according to a total lagrangian formulation concerning nonlinear grid deformation (Fig. 3).

The idea of our model is to simulate the interface between Si and SiO₂ by a trap function depending on a generation/recombination model of oxygen and silicon. Thus we can distinguish between different mechanical material characteristics depending on the value of the trap function. So it can be managed that within one single grid several different mechanical models can be calculated.

At the free silicon surface oxygen diffuses into silicon and the chemical reaction transforms it to SiO₂. Because of a volume ratio of Si:SiO₂ from 1:2.2 the volume expands. At the same time the mechanical behavior changes continuously from elastic within silicon to viscous within SiO₂ which leads to the typical deformation of the silicon block (Fig. 2). The advantage of this model approach is that in contrast to conventional modeling no regridding is necessary, because the maximal volume ratio of a single grid-element is also just 1:2.2 and the grid quality can be preserved.

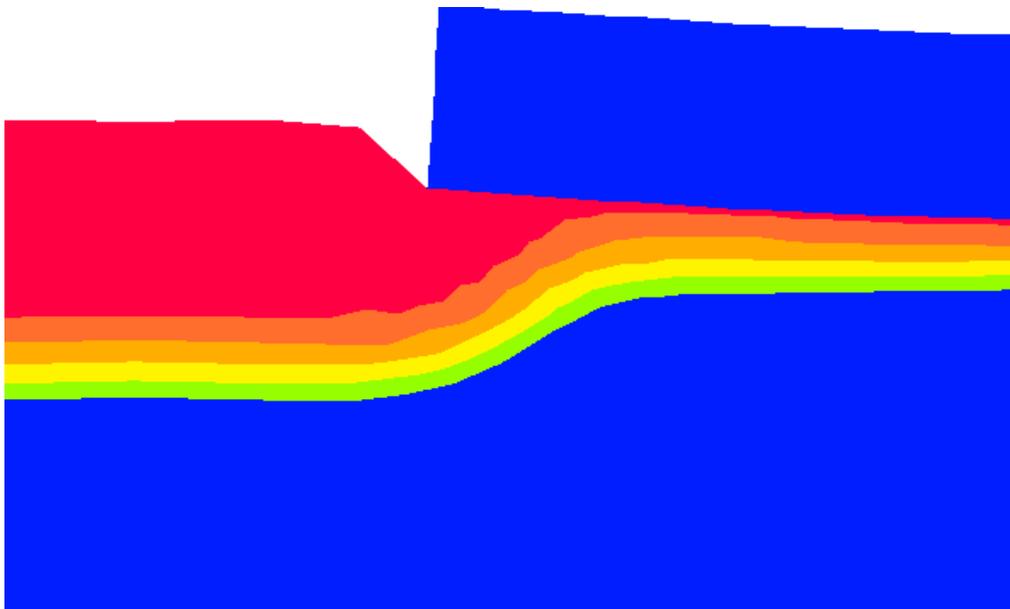


Fig. 2: Simulation result of a LOCOS

The mathematical formulation of the model:

recombination ratio of Si/O₂:

$$R_o = k_o (1 - SiO_2) \cdot O$$

diffusivity of oxygen:

$$\frac{\partial O}{\partial t} = \text{div}[D \cdot \text{grad}(O)] - 2R_o$$

generation ratio of SiO₂:

$$\frac{\partial SiO_2}{\partial t} = R_o$$

momentum conservation:

$$\frac{\partial p}{\partial x} - \mu \cdot \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = 0$$

$$\frac{\partial p}{\partial x} - \mu \cdot \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) = 0$$

continuity condition:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = k_p \cdot R_o$$

The representation of the differential equations using AMIGOS's mathematical input language:

```
MODEL Oxidation = [X,Y,P,O,SI02];
{
  source FiniteElementDiscretation(2,3)
  dt = t.t0 - t.t1;   dX = X.t0 - X.t1;
  dO = O.t0 - O.t1;   dY = Y.t0 - Y.t1;
  dSI02 = SI02.t0 - SI02.t1;
# the discretized operators
  L(xsi,eta) = [ [dNdx(xsi,eta) , NULL ]
                [ NULL , dNdy(xsi,eta)]
                [dNdy(xsi,eta) , dNdx(xsi,eta)]];
  Nabla(xsi,eta) = [[dNdx(xsi,eta)]
                   [dNdy(xsi,eta)]];
  f(x,y) = [[x,0]
            [0,y] ]; # ... function of diffusivity of oxygen
  param Dx,Dy; # ... diffusivity of oxygen

# the stiffness matrix for diffusion
  K = w_1 * detJ * Nabla(xsi_1,eta_1)^T * f(Dx,Dy) *
  Nabla(xsi_1,eta_1);
  K1 = w_1 * detJ * Nabla(xsi_1,eta_1)^T * Nabla(xsi_1,eta_1);
  Kt[i,i] = w_1 * detJ * K1[i,i];

  Ro[i] = ko*(1-SI02[i])*O[i]; # ... recombination ratio
  resO = K * O + Kt * dO/dt + Kt * Ro; # ... residual of O2
equation
  resSI02 = Kt * dSI02/dt - a * Kt * Ro; # ... residual of SiO2
equation
#----- the mechanical equations -----
-#
  param E_Si,n_SiO2,n_Si,G_Si,G_SiO2,K_Si,K_SiO2
  G = (1-SiO2) * G_Si + SiO2 * G_SiO2;
  Kappa = (1-SiO2) * K_Si + SiO2 * K_SiO2;
  D1 = [ [ 4/3 , -2/3 , 0 ] D2 = [ [ 1 , 1 , 0 ]
  [ -2/3 , 4/3 , 0 ] [ 1 , 1 , 0 ]
  [ 0 , 0 , 1 ] ]; [ 0 , 0 , 0 ]];
  D = Kappa * D2 + G * D1; m = [[1][1][0]];
# the mechanical stiffness matrices
  B(D) = w_1 * detJ * L(xsi_1,eta_1)^T * D * L(xsi_1,eta_1);
  Q = -1 * w_1 * detJ * L(xsi_1,eta_1)^T * m * N(xsi_1,eta_1);
  H[i,i] = detJ / (1.0E7-n_SiO2*1.0E10); # ... punishing term

  resM = B(D) * [[dX][dY]] + Q * P; # ... residual of momentum
  resP = Q^T * s + H * P + # ... residual of continuity
  coppl * detJ * w_1 * 1.2/(1+1.2*SiO2) * dSI02;
  gridcrit = N(xsi_1,eta_1) * dSI02; # ... the grid criterion
# ... the total residual vector to be solved for
  residuum = [[resM][resP][resO][resSI02]];

```

Fig. 3: The modeling equations and their formulation within AMIGOS's input language

4. Conclusion

With AMIGOS we have developed a powerful model development tool which supports the major interests of numerical engineering. The consequent progress in semiconductor device fabrication makes it necessary that simulation tools have to become increasingly flexible to keep up the pace of advance. First steps are taken to fulfill these requirements.

References

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