

## Three-Dimensional Transient Electro-Thermal Simulation

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### Abstract

*We present a program package based on finite elements for two- and three-dimensional analysis of interconnect structures. Thereby, triangular and tetrahedral grid elements with quadratic shape functions are used. Two preprocessors allow a layer-based input of the simulation geometry and the specification of the boundary conditions. The main program calculates amongst other things the distribution of the electric potential, the temperature and the current density. It can be applied for optimization of interconnect structures as well as for studies to verify the reliability of interconnects, as phenomena like electromigration are closely related to temperature and current density. As application example the analysis of a contact chain structure is presented.*

### Introduction

With increasing element density of deep submicron integrated circuits not only the extraction of resistances and capacitances of interconnect structures, but also the analysis of thermal effects gains importance, because the observed temperatures and current densities get closer to the physical limits. The knowledge of current density and temperature distribution in the wiring structure is important to prevent electromigration. To ensure circuits' reliability, careful investigations during the design phase are necessary, because experimental measurements of these physical effects are often expensive in terms of time and costs, difficult, or even impossible. For this purpose we have developed a two- and three-dimensional simulation tool for additional electro-thermal analysis of VLSI interconnect structures.

The largest TCAD commercial vendors present a wide range of solutions for interconnect simulations. These tools (e.g. [1, 2, 3]) have user-friendly and task-oriented interfaces, but still lack some of the features we have incorporated.

### Mathematical Models

For the numerical calculation of Joule self-heating effects two partial differential equations have to be solved.

$$\operatorname{div}(\gamma_E \operatorname{grad} \varphi) = 0 \quad (1)$$

gives the electric potential  $\varphi$  and needs to be solved only inside domains of conductive material.  $\gamma_E$  denotes the electric conductivity. Then the power loss density  $p$  is obtained by computing

$$p = \gamma_E (\operatorname{grad} \varphi)^2. \quad (2)$$

The heat conduction equation is solved to obtain the temperature distribution

$$c_p \rho_m \frac{\partial T}{\partial t} - \operatorname{div}(\gamma_T \operatorname{grad} T) = -p. \quad (3)$$

$\gamma_T$  represents the thermal conductivity,  $c_p$  the specific heat and  $\rho_m$  the mass density. The temperature dependence of the conductivities is modeled by

$$\gamma(T) = \frac{\gamma_0}{1 + \alpha(T - T_0)}, \quad (4)$$

where  $\gamma_0$  is the thermal or electrical conductivity at the reference temperature 300 K and  $\alpha$  is the temperature coefficient of the specified material.

### The Program Package SAP

The program package SAP consists of 6 modules. The simulation is performed with the tool STAP (Smart Thermal Analysis Programs [4]) which uses the finite element method for the calculation of electric potential and temperature distributions. Fig. 1 shows the main tools of the package SAP and displays the data-flow.

The layout of the interconnect structure can be imported from CIF or GDSII files, or can be created interactively with a graphical layout editor [5]. The geometry can be defined either directly from the layout by specifying layer thicknesses, or by a rigorous topography simulation [6, 7].

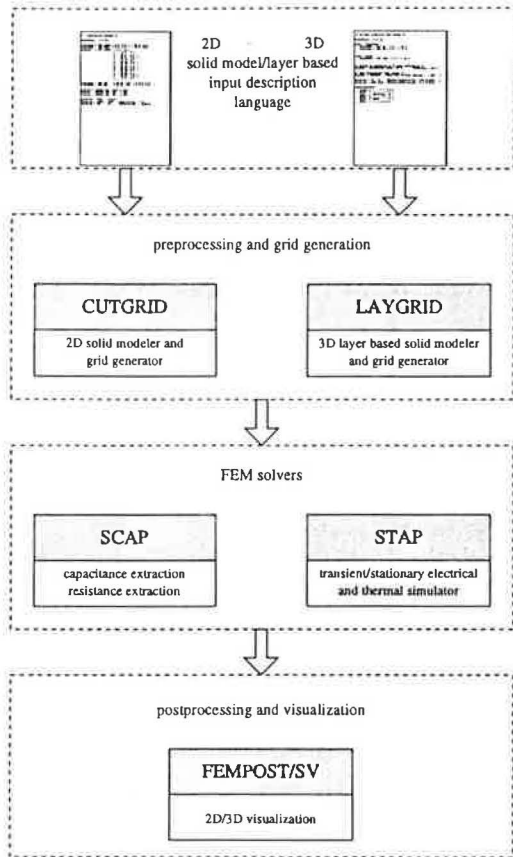


Fig. 1: The Smart Analysis Programs

Furthermore, the program package includes two preprocessors, one for two-dimensional applications (CUTGRID [8]) the other for three-dimensional applications. The preprocessor LAYGRID [9] allows a layer-based input of the simulation geometry and the specification of the boundary conditions. We use tetrahedral grid elements with quadratic shape functions for our layer-based grid generation method and utilize the possibility of refinement for the area of interest. The linear system is solved with the preconditioned conjugate gradient method. A compressed matrix format for the sparsely occupied stiffness matrix is used to achieve an efficient utilization of computer memory. In the transient thermal simulation mode the evolution of the temperature distribution in the modeled structure is calculated with Backward-Euler time discretization. Two postprocessors completes the powerful program package, whereby the visualization tool SV is based on VTK [10].

## Application Example

A contact chain test structure, commonly used for contact resistance determination is analyzed for the pur-

pose of optimization. The lateral width of the simulation domain is 1.5 times the thickness of the n+ doped silicon substrate. At the top and the bottom of the simulation domain the temperature is fixed at 300 K, and the current density is enforced due to a device specific reference current, as a current step function at time  $t_0 = 0^+$ . The results of the transient simulation are presented in Fig. 2 (temperature versus time) with the corresponding temperature distribution in Fig. 3 and the visualization of the current density (Fig. 4).

The rear half of the contact chain structure is shown in Fig. 3, which consists of two rectangular aluminium contacts above a homogeneous n+ doped silicon substrate. The four snap shots at different times show the movement location of the hottest spot in the substrate from close to the contact (Fig. 3(a), after 10 ns) to the inner part of the n+ region (Fig. 3(b), (c)). In Fig. 3(d) (after 140 ns) the two hot spots already have enlarged into the inmost part of the n+ region and they get bigger and closer. During the next few hundreds nanoseconds this process continues until one enlarged, elliptic hot spot is reached in the middle of the n+ region. Although it's obvious, that the contacts are cooling the neighboring parts of the n+ doped silicon substrate, the shape of the temperature distribution heavily depends on the size of the contacts. Decreasing the contact size (with constant length of the n+ region) reduces the cooling effects of the aluminium and the hot spots would lay beyond the contacts. The transient thermal mode is needed, because on one hand side the static calculation of the temperature distribution gains values beyond the actual values and on the other hand side the adiabatic evaluation of the distribution leads to values above the actual values.

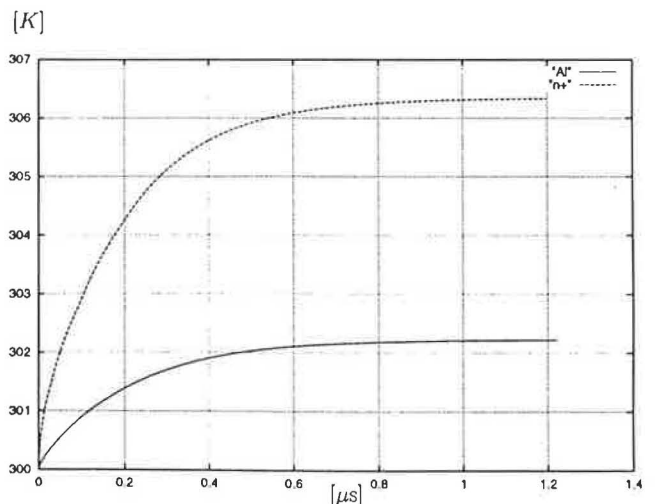


Fig. 2: Temperature versus time of the hottest spot in the aluminium contact and in the n+ doped silicon substrate

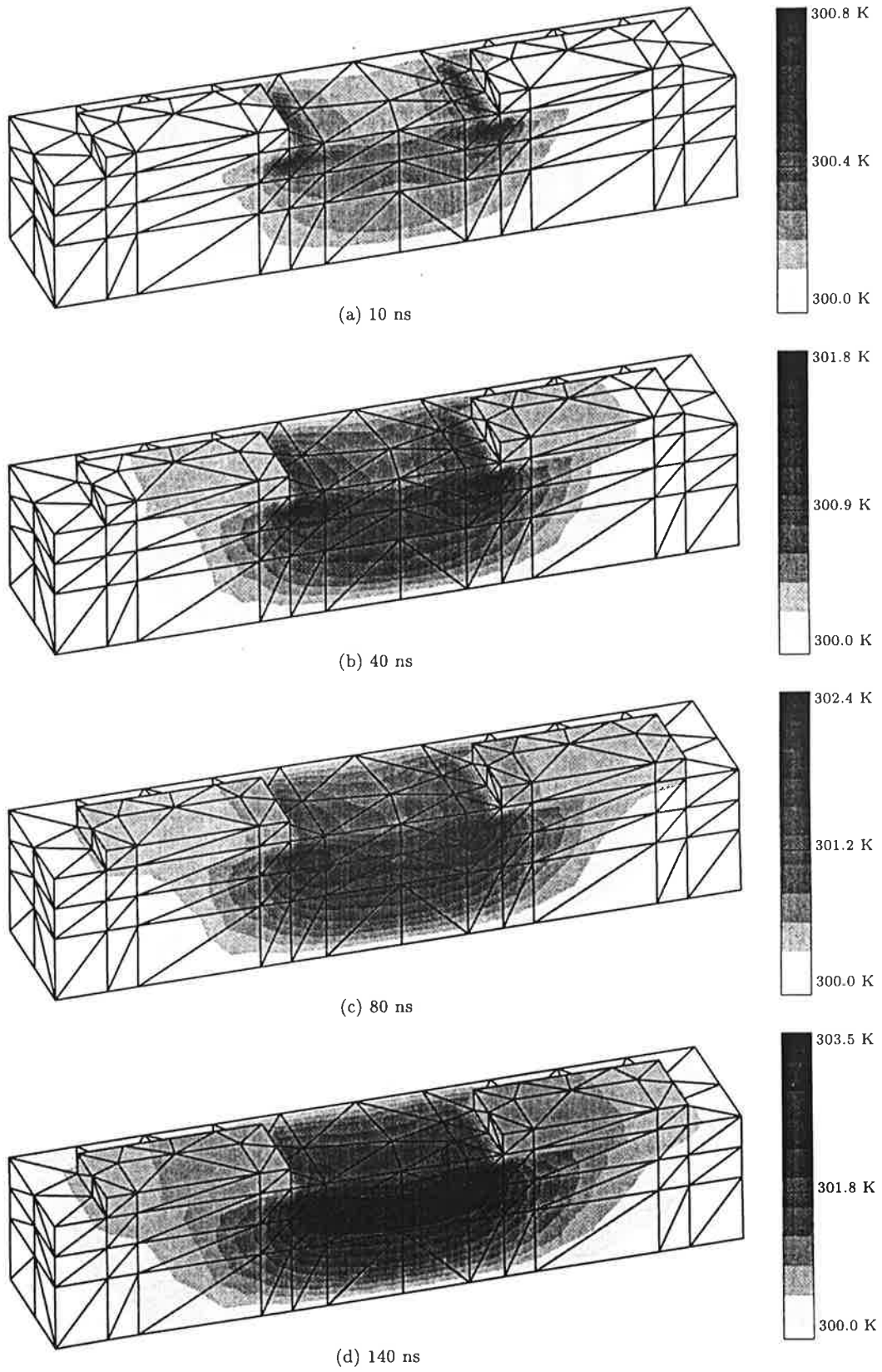


Fig. 3: Temperature distribution after 10 ns, 40 ns, 80 ns and 140 ns

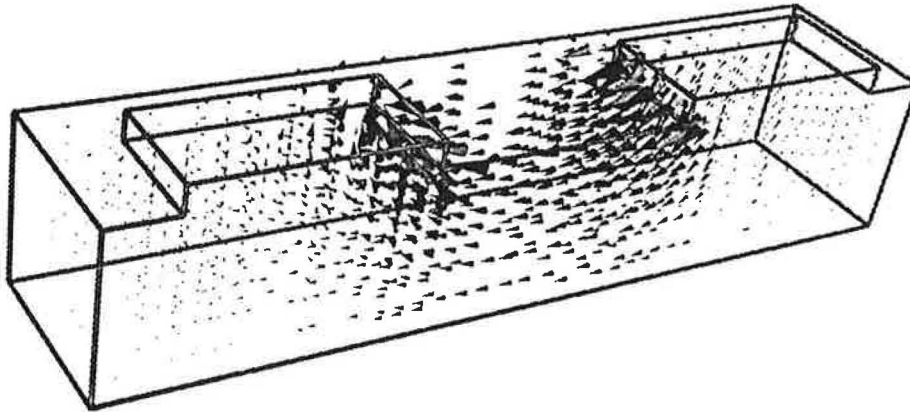


Fig. 4: Current density in the rear half structure

The temperature of the contact and the n+ region is presented in Fig. 2, and as expected it raises from 300 K to the temperature of thermal equilibrium. Obviously the temperature of the n+ region becomes higher than the temperature at the contact because of the higher resistivity of the substrate and the chosen ratio between the length of the n+ region ( $5.2\mu\text{m}$ ) and the contact size ( $1.40\mu\text{m}$ ). Thus the spot in the n+ region is not below the edge of the aluminium contact.

## Conclusion

We have described a finite element based simulation package for analysis of two- and three-dimensional interconnect structures. We have demonstrated that our package allows the analysis of transient thermal effects, in cases where neither the static nor an adiabatic calculation is feasible. The program has been tested with a large number of applications and is freely available ([www.iue.tuwien.ac.at](http://www.iue.tuwien.ac.at)).

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