

INVESTIGATION OF THERMO-MECHANICAL STRESS IN MODERN INTERCONNECT LAYOUTS

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We present a combination of transient electro-thermal simulations of three-dimensional interconnect structures and the calculation of their coupled intrinsic thermo-mechanical stress distributions. For the numerical solution of the electro-thermal as well as the thermo-mechanical stress problem, we apply the finite element method. A practical example is presented where the temperature and the pressure distribution at different times have been investigated.

Keywords: *Finite element method, interconnect analysis, electro-thermal simulation, stress simulation*

1 Introduction

The enhancements in state-of-the-art integrated circuit density and design have shown that interconnects are becoming the dominant factor determining system performance and power consumption. Interconnect reliability due to electromigration and thermal effects is a serious design issue especially for long signal lines.

Experimental results indicate that Joule heating can strongly impact the magnitude of the maximum allowed temperature of the global lines despite negligible changes in chip power density [1].

The high temperature gradients in modern interconnect structures are known to be a significant electromigration promoting factor [2]. Furthermore, a thermal expansion mismatch between the metal and the passivation layer causes additional mechanical stress which plays an important role in the development of electromigration failure mechanisms [3, 4].

The confinement of the metal lines by the passivation layer is essential in controlling the characteristics of the thermal stresses and their relaxation behavior.

With decreasing line dimensions the confinement effect is enhanced and the stress level can increase sufficiently to cause void formations.

In this work we combine transient electro-thermal models with the standard formulation of the thermo-mechanical stress problem in order to study the development of mechanical stresses during different operating conditions of complex interconnect structures.

2 Mathematical Models

2.1 Electro-Thermal Simulation

The electro-thermal simulation is performed with the tool STAP (Smart Thermal Analysis Program [5]) which uses the finite element method for the calculation of the electric potential and temperature distribution.

For the numerical calculation of Joule self-heating effects [5, 6], two partial differential equations have to be solved. The first one describes the electric subproblem

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

The electric potential φ needs to be solved only inside domains composed of electrically conducting material (γ_E represents the electrical conductivity). On the surface of the conductors three types of boundary conditions are allowed:

- Dirichlet – a constant potential is specified;
- Neumann – a constant current density is specified; and
- Floating potential – the total current is specified and the potential is forced to be the same all over the boundary area.

The next step is to compute the power loss density p_D described by

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

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Then the heat conduction equation has to be solved to obtain the distribution of the temperature T

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

Here γ_T represents the thermal conductivity, c_p the specific heat, and ρ_m the mass density.

The temperature dependence of the thermal and electrical conductivities are modelled with second order approximations:

$$\gamma(T) = \gamma_0 \frac{1}{1 + \alpha(T - T_0) + \beta(T - T_0)^2}. \quad (4)$$

Here γ_0 is the electrical or thermal conductivity at a temperature T_0 of 300 K, α and β are the linear and quadratic temperature coefficients.

This makes the problem nonlinear. Since the nonlinearity is relatively weak, a simple iterative relaxation method is used which quickly converges to the solution, usually after 3-6 iterations.

2.2 Thermo-Mechanical Stress Simulation

The thermo-mechanical stress simulation is carried out with the program package FEDOS (Finite Element Diffusion and Oxidation Simulator [7]). FEDOS is a three-dimensional finite element framework which is also able to solve mechanical stress problems.

The stress problem is based on the fundamental equation

$$\operatorname{grad}(\tilde{\sigma}) = 0. \quad (5)$$

The stress tensor $\tilde{\sigma}$ can be written in the form

$$\tilde{\sigma} = D(\tilde{\varepsilon} - \tilde{\varepsilon}_0) + \tilde{\sigma}_0, \quad (6)$$

where D is the so-called material matrix which depends in the elastic case only on Young's modulus E and Poisson's ratio v . Furthermore, $\tilde{\varepsilon}$ is the strain tensor and $\tilde{\sigma}_0$ is the residual stress tensor.

The residual strain tensor $\tilde{\varepsilon}_0$ is linear proportional to the temperature T

$$\varepsilon_0 = \alpha_m T, \quad (7)$$

where α_m is the thermal expansion coefficient for the respective material.

After the finite element discretization of the continuum [8], we obtain a linear equation system for the mechanical problem

$$K\vec{d} = \vec{f}. \quad (8)$$

Here K is the so-called stiffness matrix, \vec{d} is the displacement vector and \vec{f} is the force vector.

The force vector on an element depends on the residual strain tensor and on temperature

$$\vec{f}^e = -B^T D \tilde{\varepsilon}_0 V^e. \quad (9)$$

Here B^T is a geometry matrix [8].

After solving the linear equation system (8) we obtain the displacement vector. Since the strain is the first derivative with respect to displacement the stress can be determined with (6).

With the stress tensor the pressure can be determined by using the formula

$$p = -\frac{\operatorname{Trace}(\tilde{\sigma})}{3} = -\frac{\sigma_{11} + \sigma_{22} + \sigma_{33}}{3}. \quad (10)$$

3 Representative Example

Our model has been applied for the analysis of a three-dimensional interconnect layout as displayed in Fig. 1. In this structure the bottom layer material is silicon (Si). Above the silicon layer there is a silicon dioxide (SiO_2) layer, where two copper (Cu) lines are embedded. As usual, between the copper lines and the silicon dioxide there is a very thin titanium nitride (TiN) passivation layer. This passivation layer prevents the diffusion of copper into the silicon dioxide during the manufacturing process.

As shown in Fig. 1, the silicon dioxide layer and the copper lines are covered by a silicon nitride (Si_3Ni_4) layer which separates the next upper located silicon dioxide layer from the lower one.

In the second upper silicon dioxide layer three copper lines are embedded. These three copper lines are transverse compared to the two subjacent copper lines. This upper silicon dioxide layer is also covered with silicon nitride. On top of the layout is a third silicon dioxide layer.

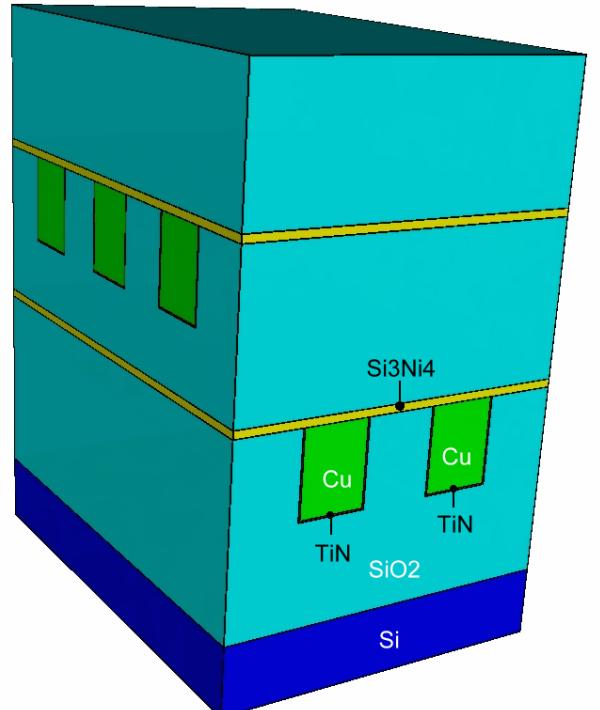


Figure 1: Representative interconnect layout.

In Fig. 2 which is a cut through Fig.1, is shown why we talk about an interconnect structure. As evident from Fig. 2 an upper transverse copper line is interconnected with a lower copper line. The other two copper lines are also interconnected in a similar way.

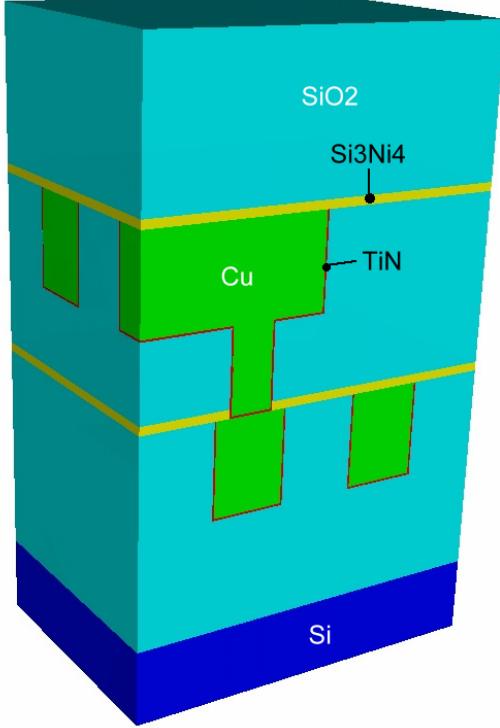


Figure 2: Cut through the interconnect layout.

4 Simulation Results

4.1 Temperature Distribution

If we apply the electro-thermal model from Sec. 2.1 to our interconnect example, we obtain the temperature distribution in the structure. For the analysis the electric and thermal conductivities given in Table 1 are used.

Due to Joule self-heating the hottest regions are around the active copper lines. This is the reason why after a time of 9×10^{-5} s the highest temperature (371 K) is in the inner layers which are surrounded by the copper conductors as shown in Fig. 3.

The relatively high thermal conductivity of copper cause that the temperature values in the copper lines are rather uniform, and so they are not included in Fig. 3.

Fig. 4 shows that, at time 9×10^{-5} s, the temperature distribution in the structure is nearly the same like in Fig. 3 (3×10^{-5} s), but due to self-heating the maximum temperature has increased to 403 K, which is 22 K higher.

Table 1: electric and thermal conductivities at 300K

	Cu	Si	SiO ₂	Si ₃ Ni ₄	TiN
γ_E [S/m]	$5,26 \times 10^7$	0,0	0,0	0,0	$1,66 \times 10^5$
γ_T [W/mK]	400,0	1,35	1,39	12,07	48,25

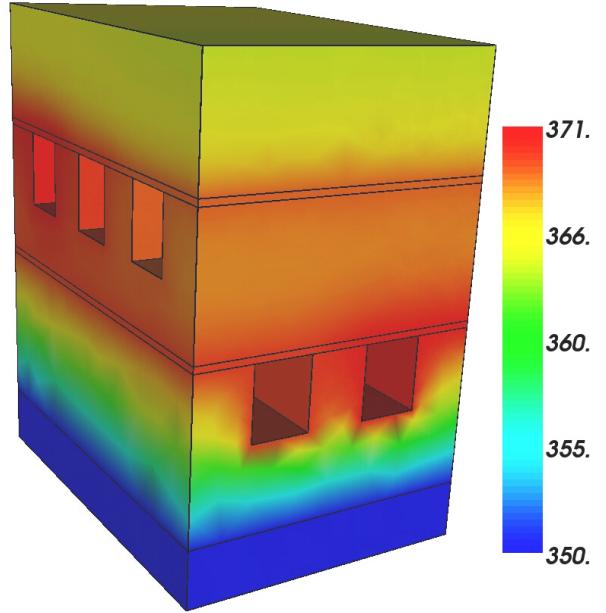


Figure 3: Temperature distribution in the silicon dioxide (SiO₂) and silicon nitride (Si₃Ni₄) layers in Kelvin [K] at time 3×10^{-5} s.

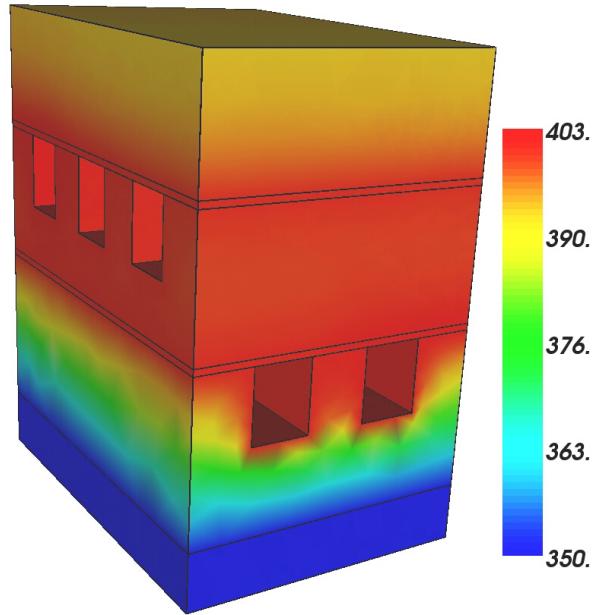


Figure 4: Temperature distribution in the silicon dioxide (SiO₂) and silicon nitride (Si₃Ni₄) layers in Kelvin [K] at time 9×10^{-5} s.

4.2 Pressure Distribution

With the obtained temperature distribution we can set up the mechanical problem as described in Sec. 2.2.

For the simulation Young's modulus E, Poisson's ratio v, and the thermal expansion factor α_m given in Table 2 are used. As applied mechanical boundary conditions the bottom surface is fixed and the other surfaces are free.

Table 2: Mechanical parameters

	Cu	Si	SiO ₂	Si ₃ Ni ₄	TiN
E [GPa]	115	180	73	380	600
v [-]	0,34	0,22	0,17	0,27	0,25
α_m [10 ⁻⁶ /K]	17,7	2,7	0,55	3,3	9,4

The pressure distribution is interesting for electromigration because the risk of electromigration is increasing with larger pressure. In Fig. 5 which shows the simulation results of the pressure distribution in the copper lines and their interconnects at time 3×10^{-5} s, it can be seen that the largest pressure (800 MPa) develops at the bottom of the interconnects.

At time 9×10^{-5} s, caused by the higher temperature in the structure, the maximum pressure in the inter-

connect structure is increased to 1150 MPa with nearly the same distribution as in Fig. 5.

5 Conclusion

We have simulated a coupled electro-thermal and a thermo-mechanical problem of a realistic interconnect structure. The hottest regions in the structure are around and between the active copper lines as result of their power loss. The thermal mismatch loads the thermo-mechanical problem, and the temperature dependent volume expansion in the materials lead to stress. In the investigated structure the largest pressure is located at the bottom of the interconnects.

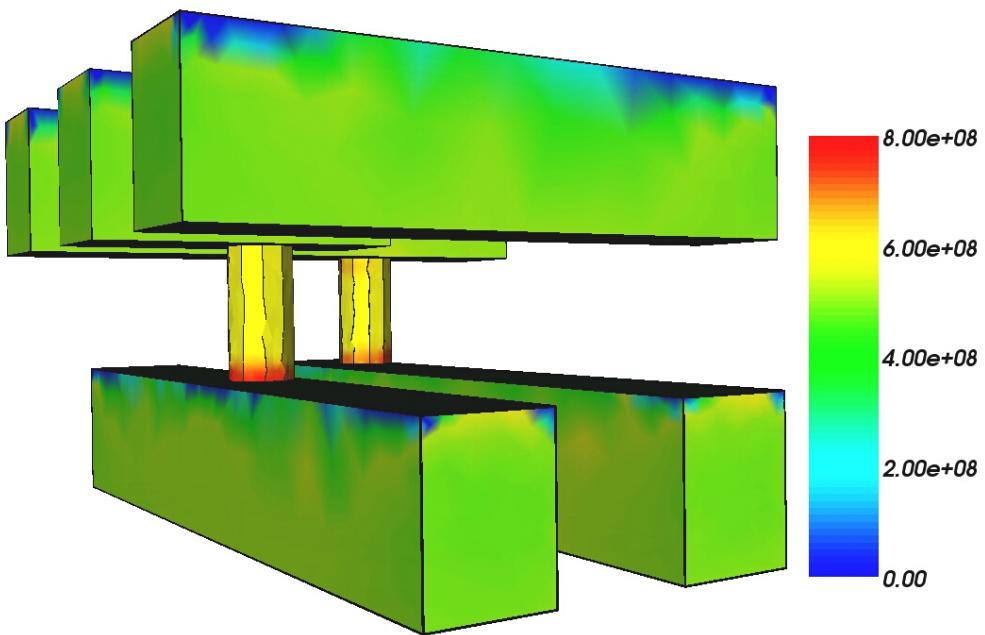


Figure 5: Pressure distribution in the copper lines and their interconnects at time 3×10^{-5} s in Pascal [Pa].

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