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# Viscoelastic Modeling of Titanium Silicidation

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Abstract

This paper describes titanium silicidation modeling using the process simulator FLOOPS. Erpimental work shows that viscoelastic models are required to fit the observed behavior. The capability to simulate a wide range of silicide examples are shown, but more experimental evidence is needed to calibrate the models.

## Introduction

Titanium silicides are widely used in the processing of vlsi and ulsi circuits but there are still very few programs that model the growth of $TiSi_2$. In two dimensions, none of the programs to date can model both the thinning at the spacer edge and the poly smile. This abstract describes the two dimensional viscoelastic model for titanium silicide growth in the process simulator FLOOPS. The model is applied to wafer curvature data to begin to determine the mechanical properties of $TiSi_2$. The type of structures that FLOOPS can simulate are also included.

## Titanium Silicide Growth Models

The model has two parts. First, we solve for the diffusion of silicon through the $TiSi_2$ to react at the titanium interface. Then we solve the flow due to the volume change of the reaction. Solving for the diffusion of silicon is done using a deal grove like reaction diffusion model[1,2,3,4]Stress dependencies in this model can be included for diffusivity, reaction rates and the mass transfer of silicon into the silicide. Which if any of these stress dependencies is correct is still under investigation.

The material deformation and flow is modeled with a viscoelastic solver which is also used for simulating oxidation. Fornara[4] used an elastic model to solve for the flow. In an earlier work[1], we used a viscous incompressible model. At the temperatures involved, 650°-800°C, oxide, polysilcon and titanium are dominated by elastic behavior. The correct model for $TiSi_2$ is still under investigation, but it is clear that there is some stress relaxation taking place. The viscoelastic solver used here is able model both elastic and viscoelastic behavior.

## Viscoelastic Calibration

The Maxwell viscoelastic model consists of a viscous element and an elastic element in series. The elastic element is characterized by Young's modulus (E) and Poisson's ratio (v). Jongste et al.[4] have measured these values for C49 $TiSi_2$ using wafer curvature measurements to be E=142 Gpa and v=0.27. The viscous element relieves the stress stored the elastic element.

In two wafer curvature studies Jongste et al.[5,6] saw significant stress relaxation. The papers present data from in-situ stress measurements during RTA of titanium and silicon multilayers. In one study[5], the Si/Ti ratio of the multilayers was varied from 1.9, 2.1 and 2.4. Stress as a function of time at a constant temperature was plotted in this study. There was relaxation for all the compositions but more relaxation for Si/Ti ratios > 2. Using this data we can start to calibrate the viscosity in our model by simulating the wafer curvature. This is done by simulating the whole wafer with the viscoelastic solver. Figure 1 shows relaxation data at 525° C for a Si/Ti ratio of 2.1, along with some simulated curves. To fit the amount of relaxation with a linear viscosity requires an extremely low value of approximately 1.5e13 poises. The curve of the simulation is incorrect and the stress over relaxes. To try and better fit the data an Eyring stress dependent viscosity was used. There are two parameters needed for this model - the low stress viscosity and the nonlinear activation volume. Unfortunately neither of these parameters is known. A low stress viscosity of 1e20 poise is picked and the nonlinear activation is varied to try and fit the data. Obviously there are many choices for the low stress viscosity and more experimental evidence is needed. There are two other interesting things to note about this data. One is that the viscosity needed to fit a Si/Ti ratio of 1.9, ~1e16 at 625 C, while higher than Si/Ti ratio > 2 is still much lower than the viscosity of oxide at these temperatures. Second is that the method of relaxation seems to be the diffusion and precipitation of Si. This will probably affect the growth kinetics. One note on the applicability of this data to silicides grown from deposited Ti on substrate or poly silicon is that Norstrom et al.[7] found chains of silicon precipitates in the middle of narrow lines that were silicided with titanium. The lines exhibited the characteristic bowing seen on narrow lines. More work needs to be done but it is clear that a viscoelastic model is needed to accurately model the stress relaxation seen in $TiSi_2$ experiments.

## Salicides and Local Interconnect Examples

We are currently able to simulate most of the interesting structures with titanium silicides. As our calibration of the viscoelastic model progresses we can begin to use these parameters on real world structures like salicides and local interconnects. This should allow us to begin to calibrate the stress dependencies in the diffusion reaction model. Figure 2 a shows a linear viscoelastic simulation of a salicide structure in a nitrogen ambient. The growth of titanium nitride is also modeled. Figure 2 b shows titanium silicide local interconnect over a field isolation region. Both of these figures do not yet match with experimental evidence. The purpose is to demonstrate the range of simulations FLOOPS can perform and how this can be used to simulate a wide range of silicide structures. The user is not required to provide seed or native meshes for either the $TiSi_2$ or TiN. When annealed these meshes are inserted into the structure.

## Conclusion

A nonlinear viscoelastic solver has been applied to modeling titanium silicide experimental results. It is found that the stress relaxation is significant and the viscous component of $TiSi_2$ can't be ignored. The ability to simulate real world structures has also been shown.

## References

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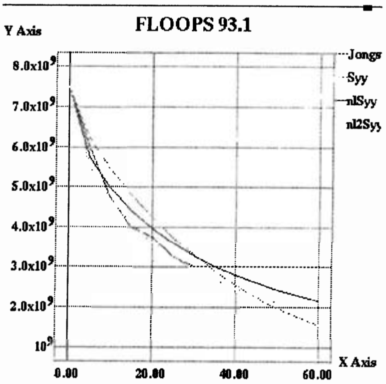

Figure 1: Stress relaxation data from Jongste[1] and simulation results: linear viscosity ($S_{yy}$) 1e13 poises, nonlnear viscosity ($nlS_{yy}$) u=1e16 poises Vd=65e4 $A^3$ and ($nl2S_{yy}$) u=1e20 poises Vd=1.1e10 $A^3$.

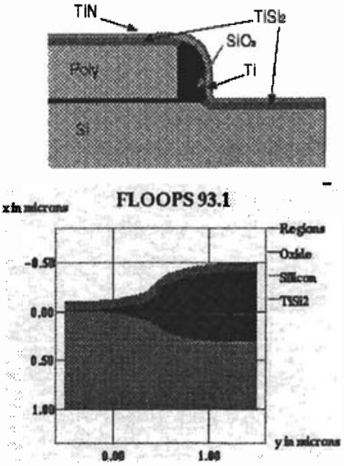

Figure 2: Silicide examples a) salicide and b) local