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Prediction of porous dielectric line wiggling phenomenon with metallic hard mask: From simulation to experiment

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The patterning of narrow trenches in porous SiOCH with a metallic hard mask can lead to the undulation of the dielectric lines between the trenches, also called wiggling. This phenomenon is attributed to the relaxation of the residual stress of the highly compressive hard mask by deforming the mechanically weak porous dielectric. This work analyses the parameters (titanium nitride stress and thickness, lines width and height, and materials Young modulus) potentially responsible for dielectric lines undulations using finite element mechanical modeling. These simulations are experimentally validated. © *2014 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4882080]

Copper/ultra-low-k interconnects are necessary for integrated circuit (IC) performance but lead to challenges in process manufacturability and scalability. Today porous SiOCH combined with metallic hard masking strategy is an integration of choice for advanced interconnects.[1,2] However, with the constant downscaling in device dimensions, etching process steps are facing new issues. Indeed, patterning of sub-100 nm porous SiOCH (p-SiOCH) trenches using a metallic hard mask approach leads to a line undulation phenomenon, also called line wiggling.[3] We were the first to report the wiggling of porous dielectric lines patterned with a titanium nitride hard mask. The wiggling phenomenon is attributed to the low mechanical property of the dielectric material coupled to the high compressive stress of the metallic hard mask. This mechanical phenomenon can lead to voids formation during metallization and could become a real issue for interconnects fabrication in future technological nodes.[4] To study this issue, we evaluate hard mask stress, hard mask thickness, porous SiOCH film thickness, and titanium nitride and porous SiOCH young moduli, envisioned as potential parameters responsible for wiggling. Finite element mechanical simulations are performed using the commercial code ANSYS™ as detailed in a previous study.[3] The buckling analysis is for bifurcation buckling using a linearized model of elastic stability. The simulated structure used for buckling analysis consists of a 1 μm long line with the typical stack of the interconnect at the 32 nm technological node: SiCN/porous SiOCH (k = 2.5, porosity 25%)/SiO_2/TiN), represented Figure 1.

To simulate an infinite line, the longitudinal displacement in constrained to 0 at each ends of the line. The mechanical properties (coming from the literature[5]) and residual stress of materials used in our structure are summarized in Table I.

The matrix of stiffness and the matrix of stress stiffness are calculated from this structure based on iterative calculation of equilibrium state. From buckling analysis, we can extract the coefficient by which we have to multiply the matrix of stress stiffness [S] to reach the first buckling Eigen mode. This so-called buckling coefficient is critical when it lies under unity.[3]

The effect of the residual stress and layers thickness on the buckling of dielectric lines is simulated as a function of the dielectric line width (see Figure 2(a)). Each curve shown in this graph corresponds to a buckling coefficient of 1 and separates the line width/residual stress plan into two areas. For each parameter, the left hand side of the plan delimitated by the curve corresponds to a buckling coefficient lower than 1 (wiggling), while the right hand side corresponds to a buckling coefficient higher than 1 (no wiggling). As shown in Figure 2(a), for a 45 nm-thick TiN layer having a highly compressive residual stress (−2200 MPa), no wiggling is expected for lines wider than 35 nm. Reducing the titanium nitride thickness down to 15 nm relaxes the limit for wiggling down to 20 nm wide features. With less compressive TiN (−750 MPa) and similar thickness (45 nm) no wiggling is expected until less than 20 nm width, evidencing that titanium nitride residual stress and its thickness play a key role on the line undulation.

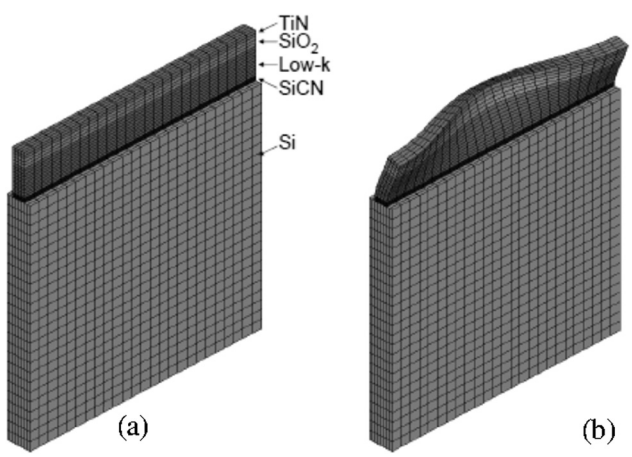

FIG. 1. Example of simulated stack before (a) and after deformation calculation (b) C032 Metal 1.

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TABLE I. Mechanical properties and residual stress of materials used in the investigated patterned structures.

Materials	E (GPa)	Stress (MPa)
TiN	79	−750/−2200
SiO_2	75	100
Porous SiOCH	6	100
SiCN	67	−300

The effect of the porous SiOCH line height on the wiggling phenomenon is also simulated by varying the porous SiOCH thickness between 20 and 300 nm for a highly compressive TiN mask (−2200 MPa). Figure 2(b) shows that when the porous SiOCH line height increases, the line width for which the wiggling phenomenon is observed increases as well, indicating that the wiggling also depends on the porous SiOCH line height.

The effect of the titanium nitride young modulus on the line wiggling, represented Figure 2(c), suggests that titanium nitride Young modulus variations of 200 GPa have a low impact on the wiggling since it is only allows a 5 nm relaxation on the line width before line wiggling. Similar results can be drawn for the impact of the porous SiOCH young modulus (not shown here).

These simulations show that the hard mask properties (residual stress and thickness) are the main factors responsible for dielectric line wiggling. But this phenomenon also depends of the porous SiOCH line height and line width at the second order. On the contrary, titanium nitride and porous SiOCH young moduli have only "a very small impact" on the wiggling compared to the impact of the titanium nitride stress and thickness.

To validate these simulation results, experiments have been performed on 300 mm wafers patterned using the stack previously described: 20 nm SiCN/290 nm porous SiOCH (25% porosity)/40 nm SiO_2/25 nm TiN deposited by physical vapor deposition. Different titanium nitride stresses have been investigated: high (−2250 MPa) and low (−750 MPa) residual stress. After line photolithography, the resist is trimmed during the anti-reflection coating and TiN opening steps using chlorine-based etching processes. After photoresist strip, the titanium nitride line patterns are transferred into SiO_2 and porous SiOCH with a C_4F_8-based capacitively coupled plasma in a LAM Versys Flex45^{TM} reactor.

The profile evolution obtained after etching is presented Figure 3 showing that for a high residual stress, the line starts to wiggle at 45 nm (Figure 3(c)) while using a lower titanium nitride stress relaxes this line undulation down to 30 nm (Figure 3(a)). These observations are in good agreement with the previous simulations, showing that lowering the titanium nitride residual stress relaxes the limit of the line undulation. We can notice in Figure 3 that the line buckling tends to be collective with either in phase or out of phase buckling of adjacent lines. Such behavior has already been reported in the literature for elastic materials patterned by soft lithography. Substrate deformation leads to coupling between lines which results in collective buckling.[6] In our case, the same mechanism can explain the collective lines buckling observed in Figure 3.

Figure 4 represents a superposition of the simulation and experimental results previously described for line wiggling for different titanium nitride residual stress as a function of the line dimension. This comparison shows that for high titanium nitride residual stress (−2250 MPa), there is a good match between simulation and experiments. For a low titanium nitride residual stress (−750 MPa), the wiggling appears for lines 10–15 nm wider in the experiments than in the simulations.

Different assumptions can be raised to explain this difference.

The first one is the titanium nitride stress modification during the different etching steps (hard mask opening, cleaning and porous SiOCH etching). A measurement of the titanium nitride residual stress on blanket wafer performed after exposition of the titanium nitride to the different etching processes reveals that for both titanium nitride investigated (high and low stress), the residual stress remains constant whatever the plasma etching chemistry. This indicates the

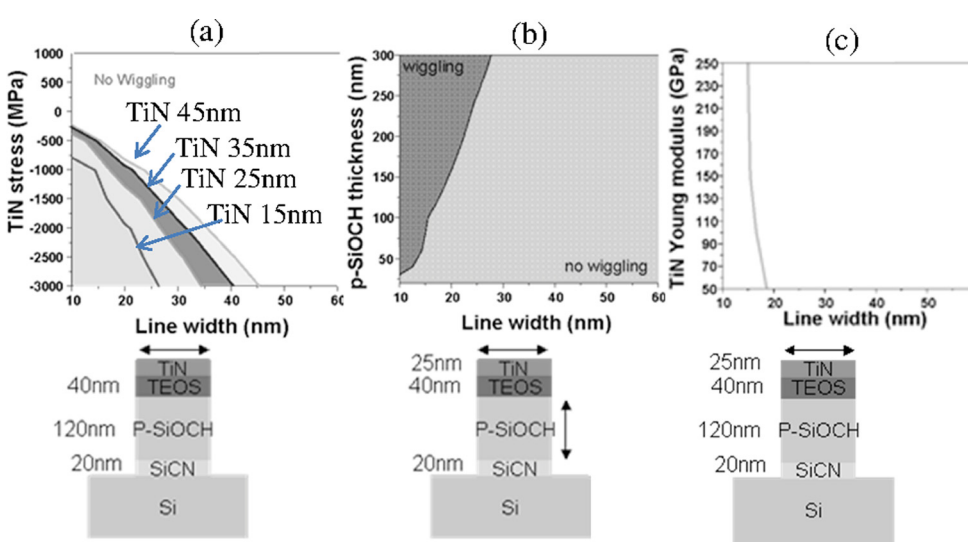

FIG. 2. Evolution of buckling coefficient as function line width, titanium nitride stress and thickness (a), porous SiOCH height (b), and titanium nitride Young modulus (c).

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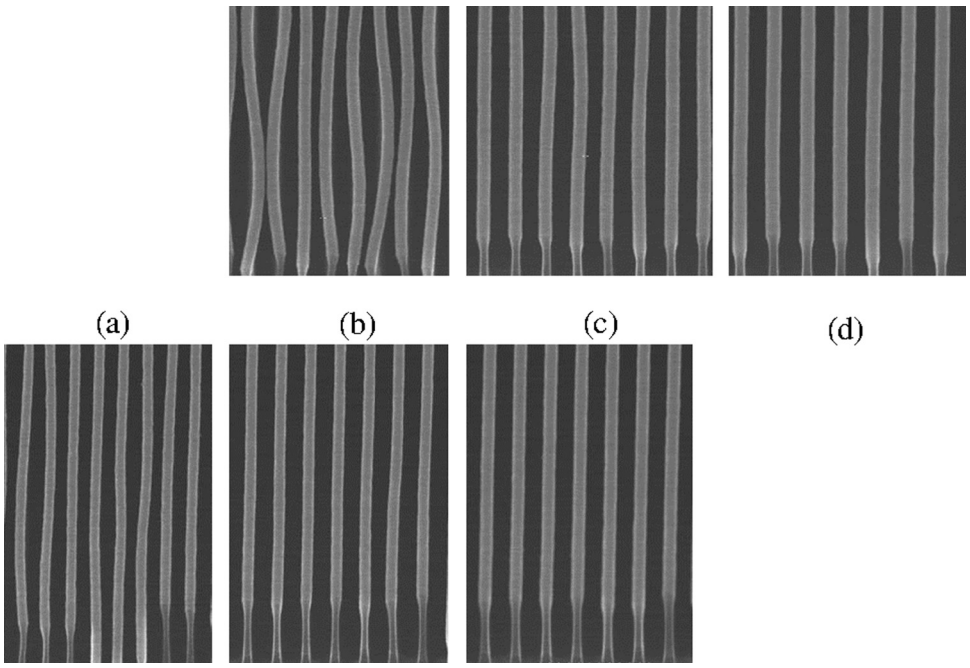

FIG. 3. Profile evolution of porous SiOCH line after etching using residual titanium nitride hard mask stress of −2250 MPa (top) and −750 MPa (bottom) for different line dimension (a) 30 nm, (b) 35 nm, (c) 45 nm, and (d) 50 nm.

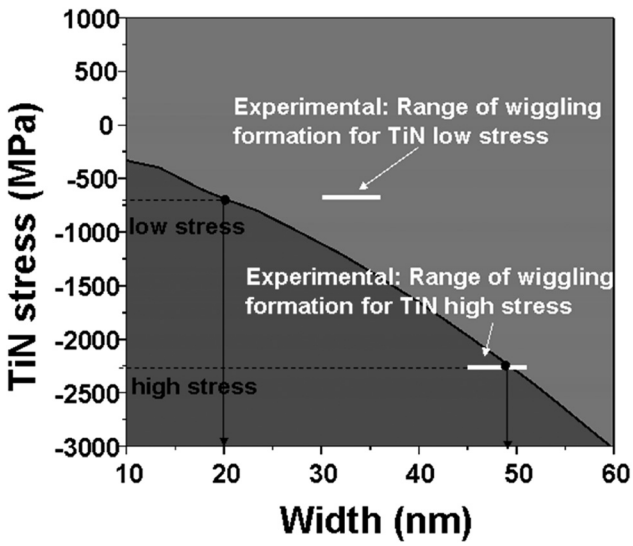

FIG. 4. Comparison of the line wiggling formation between simulation prediction and experimental results for different titanium nitride residual stress as a function of the line dimension.

titanium nitride stress is not significantly altered by the etching processes and the difference between simulation and experiments cannot be explained by variations of the titanium nitride residual stress along the processes.

The second assumption is the effect of the porous SiOCH film modification during etching, modifying its properties.[7] However, previous simulations demonstrated that only the porous SiOCH film thickness plays a significant role in the line wiggling, while the porous SiOCH properties playing a role but at third order. Therefore, even if the porous SiOCH film modification can explain a part of the difference observed between simulation and experiments it cannot explain the shift of 10–15 nm line dimension for wiggling between prediction and experimental data.

The third assumption is an incorrect modeling of the structure. In fact, cross section observations performed after etching using different titanium nitride residual stress (high and low) show an important bowing in the line profiles (Figures 5(a) and 5(b), respectively).

Our simulations did not take into account this bowed profile. With a bowed profile, the titanium nitride line width is larger than the porous SiOCH one at mid-height, and the

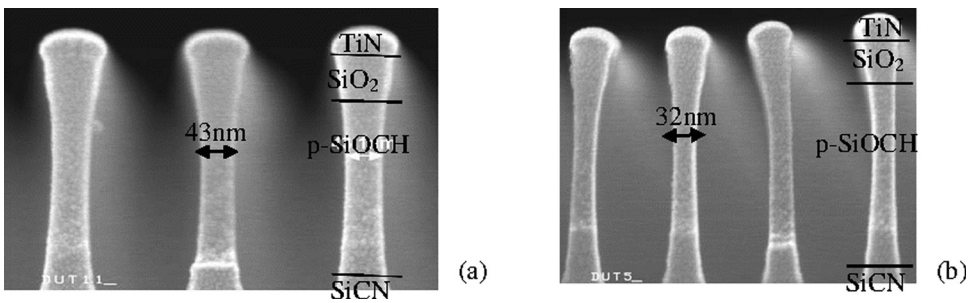

FIG. 5. Profile evolution of porous SiOCH after etching when the line undulation is first observed for a line dimension of 45 nm (using high TiN stress (−2250 MPa)) (a) and 35 nm (when using low titanium nitride stress (−700 MPa)) (b), respectively.

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dielectric line is not as stable as a dielectric line with the same width as the titanium nitride hard mask. Complementary simulations (not shown here) realized with a titanium nitride line width twice larger than porous SiOCH line revealed that line undulation appears for lines 5 nm wider compared to simulation with a vertical profile (titanium nitride line dimension equals to porous SiOCH line). Given the measurement error of the line width in cross section measurements, the difference of line wiggling determined by simulations and obtained experimentally can be explained by the cumulative effect of the porous SiOCH film modification and the bowed profile formation during line etching.

In this Letter, we showed that the TiN layer stress and thickness are the main parameters impacting the line wiggling. On a second order, the wiggling is impacted by the dielectric line height. Simulations are in good agreement with experimental data when using high residual stress. Using a lower titanium nitride residual stress, we observe a little shift between simulation and experiments assigned to bowed profile and dielectric film properties change, not taken into account in the simulation. All results clearly indicate we need to play on the main factor by developing a low stress hard mask to continue to implement porous SiOCH in future technological nodes. This can be achieved by playing on the metallic hard mask deposition parameters.

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