Thermomechanical Response Analysis of Lithographic Mask Structure Using Finite Element Method*

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The influence of heavy X-ray irradiation on the thermal and mechanical behavior of a silicon-tungsten (Si-W) mask structure in semiconductor microlithography was examined by numerical simulation. To approach the realistic physical conditions in X-ray lithographic exposure, a relatively large three-dimensional finite-element model with 6 480 elements and 7 760 grids was created to simulate the Si-W mask under thermal loading. The finite-element calculation was performed by using the commercially available MSC/NASTRAN program with IDEAS pre-post processor system on a powerful CONVEX C201 minisupercomputer. Investigations were focused on the temperature distributions, the thermal stress profiles, and the thermal displacement contour in the Si-W mask structure. The simulated results can provide both qualitative and quantitative information for optimal mask design to minimize in-plane thermal distortion.

Key Words: X-Ray Irradiation, Si-W Mask Structure, Semiconductor Microlithography, Finite-Element Model, Thermal Stress, Thermal Displacement, Mask Design

1. Introduction

Microlithography is the process by which geometrical micropatterns are transferred from a mask onto the wafer surface or onto the surface of a film covering the wafer.⁽¹⁾ Among various lithography methods used in semiconductor fabrication, X-ray lithography (XRL) is currently regarded as a very promising technology because of its clear potential for resolving features smaller than 0.1 μm and significant processing advantages over conventional optical lithography, such as high depth of focus, large field size, immunity to dust particles and excellent process latitude.⁽²⁾

Especially due to its extreme depth of focus and penetrating exposure wavelengths, XRL is the only mass-production lithography technique to fabricate three-dimensional microstructures with high depth-to-width aspect ratios, large structural heights, and perfectly parallel edges. Therefore, in the near future, the application of XRL will be not only to the volume manufacturing of ultra large-scale integrated (ULSI) circuits but also to the field of micromechanical engineering, which is a new fast-growing discipline concerning the development of novel microcomponents (e.g., microgear, micromotor, microactuator, micropump, acceleration sensor, etc.) for the realization of intelligent microelectromechanical system (MEMS)⁽³⁾.

Figure 1 sketches the general steps which usually form the basis of the XRL process. The imaging process is carried out by X-ray irradiation through the patterned mask onto a wafer coated with a photosensitive resist, and the developed resist serves as a template for subsequent processing steps, such as etching, electrodeposition, and ion implantation. The illustration of the basic process sequence is only a schematic one. According to the specific demands on

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Fig. 1 Typical process steps in microdevice fabrication

the final microproducts, the microfabrication process can be modified to generate various microstructures with complex geometries from a broad range of materials including ceramics, metals, and polymers. The final microdevice is fabricated by repeating the replication process many times with different masks.⁽¹⁾ The mask itself consists of a membrane of low-atomic-weight material which has a relatively high transparency to X-rays and a metallic absorbing pattern of high-atomic-weight material which has a high X-ray stopping capability.

The fabrication of X-ray mask is complicated by the fact that no thick, rigid, mask blank material which is transparent to soft X-rays is available. Therefore very thin membranes overlaid with X-ray opaque materials must be used, which have problems of thermomechanical stability. Specifically, the mask can be subjected to substantial heating and thermal stress by high-intensity X-ray sources during exposure, leading to a serious problem of mask distortion. If the magnitude of mask distortions exceeds 10% of the absorber minimum linewidth, the required mask-to-mask overlay accuracy for integrated circuit (IC)

fabrication will be degraded. Presently both synchrotron storage rings and plasma sources are being extensively used as high-power X-ray sources for lithography applications. Synchrotron radiation is generated when relativistic electrons in circular motion are deflected by a magnetic field, and it has a nearly time-constant radiation power.⁽⁴⁾ Since the synchrotron radiation reaching the mask is generally prefiltered by the grazing mirror and vacuum window inside the beamline (i.e., the radiation transport system), the maximum power on the mask is about 150 mW/cm². On the other hand, the plasma source is different in that the radiation is emitted by a high-temperature, high-density short-lived plasma, which is produced by either a high-power laser source or an electrical discharge.⁽⁵⁾ The intensity is distributed isotropically and delivered in a very short duration of 5 - 20 ns with extremely high-power pulses amounting to 10⁵ - 10⁶ W/cm².

Because the fabrication and metrology of X-ray mask are intricate, time-consuming and very expensive, it is unreasonable to use a large number of mask prototypes for conducting experiments to study the thermal-induced mask distortions during the initial stage of mask design. Thus an effective approach, such as the finite-element method, should be applied to investigate the problems early in the design process to decrease costs and shorten development time. Finite-element models have been successfully used in many fields of engineering. Such models can, in principle, be made arbitrarily accurate by dividing the model into a sufficient number of elements. In this paper, the thermoelastic response of an X-ray mask structure comprising tungsten (W) absorber on silicon (Si) substrate membrane under high-intensity X-ray irradiation was investigated by finite-element modeling. In order to obtain reasonable numerical solutions, design-oriented methodology was employed in the calculations. In other words, the models and assumptions adopted here were carefully planned in advance to approximate the practical configuration in XRL exposures. By using the commercially available MSC/NASTRAN finite-element program with IDEAS pre-post processor system, the transient behaviors of X-ray mask with respect to temperature, stress, and displacement were simulated. A powerful CONVEX C201 minisupercomputer was used to deal with the extremely large amounts of data and to save computer time. The simulation results obtained in this paper may be useful to define future specifications in the design of X-ray mask structures.

2. Formulation

The incident X-ray power is transformed into

heat energy by absorption in the mask materials, primarily due to the photoelectric effect. The temperature rise of a mask, subjected to intense soft-X-ray irradiation, depends on heat-dissipating mechanisms of thermal conduction, radiation, and convection, and then on the mutual heat transfer among a membrane, an absorber, a surrounding gas, and a wafer, as illustrated in Fig. 2. Consequently, the heat balance equation governing the temperature distribution in the mask can be expressed as follows:⁽⁶⁾

$$\frac{\partial T}{\partial t} = \frac{\phi}{\rho C} \left(\frac{\partial^2 T}{\partial x^2} - \frac{\phi}{\phi D} T \right) + \frac{H}{\rho C} - \frac{\eta \beta}{\rho C D} \left[(T + T_0)^4 - T_0^4 \right] \quad (1)$$

where T is the temperature change (K), ϕ is the thermal conductivity, ρ is the density, C is the specific heat, ϕ is the convective heat transfer coefficient, D is the thickness, H is the heat source due to X-ray absorption, η is the emissivity, β is the Stefan-Boltzmann constant ($=5.67 \times 10^{-12} \text{ W cm}^{-2} \text{ K}^{-4}$) and T_0 is the initial temperature.

As the influence of X-ray scattering is insignificant for soft-X-ray lithography, Beer's law of absorption can be applied in the calculation of mask heating.⁽⁷⁾ Assuming that the temperature variation along the film depth is uniform, the heat sources H can be written as:

$$H_m = \frac{I_0}{D_m} [1 - \exp(-\mu_m D_m)] \quad (2.1)$$

$$H_a = \frac{I_0}{D_a} \exp(-\mu_m D_m) [1 - \exp(-\mu_a D_a)] \quad (2.2)$$

$$H_p = \frac{I_0}{D_p} \exp(-\mu_m D_m - \mu_a D_a) [1 - \exp(-\mu_p D_p)] \quad (2.3)$$

where I_0 is the incident X-ray power density, and μ is the linear absorption coefficient. The subscripts m , a , and p represent the membrane, absorber, and proximity gap, respectively. The linear absorption coefficient at the wavelength of $10 \text{ \AA}$ is assumed.

Because the mask materials are extremely thin (only a few microns thick) when compared with the entire mask window size (normally several centimeters wide), the mask surface is considered to be in

Fig. 2 Schematic diagram of X-ray exposure setup and heat distribution mechanism

a state of plane stress; that is, the only nonzero stresses are σ_x , σ_y , τ_{xy} , and they are independent of the Z coordinate. Thus the displacements, u and v , in the plane are also independent of Z . Assuming that the mask materials are linearly elastic isotropic, the thermal expansion coefficient α is the same for all directions. Using Hooke's law for plane stress, we can relate the stresses to the strains ϵ_x , ϵ_y , and γ_{xy} as described below:

$$\epsilon_x = \frac{\partial u}{\partial x} = \frac{1}{E} (\sigma_x - \nu \sigma_y) + \alpha T(x, y, t) \quad (3.1)$$

$$\epsilon_y = \frac{\partial v}{\partial y} = \frac{1}{E} (\sigma_y - \nu \sigma_x) + \alpha T(x, y, t) \quad (3.2)$$

$$\gamma_{xy} = \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} = \frac{2(1+\nu)}{E} \tau_{xy} \quad (3.3)$$

In matrix form, the above equations become

$$\begin{Bmatrix} \sigma_x \\ \sigma_y \\ \tau_{xy} \end{Bmatrix} = \frac{E}{1-\nu^2} \begin{bmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & (1-\nu)/2 \end{bmatrix} \begin{Bmatrix} \epsilon_x - \alpha T \\ \epsilon_y - \alpha T \\ \gamma_{xy} \end{Bmatrix} \quad (4)$$

or

$$\{\sigma\} = [Q] \{\epsilon - \epsilon_0\} \quad (5)$$

where ϵ_0 is initial strain, E is Young's modulus, ν is Poisson's ratio, and $T(x, y, t)$ is the temperature profile on the mask surface.

3. Calculations

An X-ray mask structure with a $2\text{-}\mu\text{m}$ -thick Si membrane and a W absorber $0.8\text{ }\mu\text{m}$ thick was considered for computer simulations. The proposed layout of the Si-W mask structure is shown in Fig. 3. The Si membrane is a rectangle $6 \times 7\text{ }\mu\text{m}$, and the W absorbers ($0.25\text{ }\mu\text{m}$ minimum linewidth) comprise typical geometric features normally encountered in a practical X-ray mask, such as square pad, pillar, line and space gratings. The entire mask structure was

Mask for X-ray ($\lambda = 1\text{ nm}$) Lithography

(A) Macroscopic Cross-sectional View

(B) Macroscopic Top View

Geometry of pattern structures on X-ray mask

Fig. 3 Layout of the Si-W mask used in the calculations

assumed to be surrounded by a helium (He) environment. The thermomechanical parameters of the different materials used in the calculations are summarized in Table 1. In addition, two different X-ray sources were used in the calculations. One is a synchrotron beam with a power density of 150 mW/cm², and the other is a plasma X-ray pulse with a power density of 5×10^8 W/cm² in a very short duration of 10 ns. Table 2 shows the two cases considered, which were selected in order to simulate actual operating conditions. The assumed X-ray wavelength was 10 Å.

The analysis of heat transfer in the mask structure (a solid continuum) can be reduced by finite-element techniques to the solution of a set of equilibrium equations in which the unknowns are defined at a discrete set of points. Hence, the general equation which is solved when finite-element methods are applied to heat transfer analysis may be written in the form⁽⁸⁾

$$[K]\{q\} + [B]\{\dot{q}\} = \{P\} + \{N\} \quad (6)$$

where $[K]$ is the symmetric matrix of constant heat conduction coefficients, $\{q\}$ is the vector of temperature at grid points, $[B]$ is the symmetric matrix of constant heat capacity coefficients, $\{\dot{q}\}$ is the vector of temperature gradient, $\{P\}$ is the vector of applied heat flows which are known functions of time, and $\{N\}$ is the vector of nonlinear heat flows which depend on temperature. Heat transfer analysis with the MSC/NASTRAN program utilizes all of the normal analytical tools provided for structural analysis, the discrepancy being that the arrays $[K]$, $[B]$, $\{P\}$ and $\{N\}$ are computed from thermophysical properties, rather than from structural properties.

For transient thermal analysis, the capabilities offered by MSC/NASTRAN Solution Sequence 89 (SOL 89) were used in the present study. After the temperature distribution is obtained, SOL 24 is employed for the stress analysis by assuming zero intrinsic stress. For the microscopic model construction, three layers of elements in the thickness direction were used. Accordingly the total numbers of solid elements and grids are 6 480 and 7 760, respectively. The finite-element models used for the calculations are shown in Fig. 4.

4. Results and Discussion

When the mask is placed next to the wafer with a small gap in an exposure chamber, the heat will flow from the irradiated mask surface into the He gas in the gap and induce a free convection state. Due to the extremely small X-ray attenuation for He gas, the heat source due to X-ray absorption in the gap can be neglected. Since the static He gas boundary layer

involved has an extremely large length (up to several centimeters) compared to the much smaller proximity distance (only 40 μm), the cooling effect resulting

Table 1 Thermomechanical parameters used in the calculations

	Poisson ratio	Young's modulus $\times 10^{12}$ dyn/cm ²	Density g/cm ³	Thermal expansion $10^{-6}/^\circ\text{C}$	Thermal conductivity W/cm ² °C	Absorption coefficient $\mu\text{ m}^{-1}$	Thickness μm	Specific heat J/kg °C
Si	0.28	1.30	2.30	2.33	1.57	0.203	2.0	712
W	0.40	3.45	19.3	4.50	1.78	5.003	0.8	132
He			1.8×10^{-4}		1.5×10^{-3}	5.39×10^{-7}	40	5193

Table 2 Computational cases considered

	Case 1	Case 2
Source type	Synchrotron radiation	Plasma pulse
Power density	150 mW/cm ²	5×10^8 mW/cm ²
Exposure time	1 sec	10 ns

(a) Without He surrounding

(b) With He surrounding

Fig. 4 Finite-element models of the Si-W mask structure used in the calculations

from free convection is negligible and therefore thermal conduction from the mask through the surrounding He gas to the wafer (a heat sink with the constant temperature of 25°C) is the most important heat transfer mechanism.

4.1 Temperature and thermal stress distributions

4.1.1 Case 1 Figure 5 illustrates the transient response of temperature distribution on the mask structure for Case 1. Several distinctive temperature zones are observed in this figure, indicating the existence of temperature gradient from the region of W

Fig. 5 Temperature distribution of the Si-W mask structure irradiated by a synchrotron source with 150 mW/cm² power density for a 1-sec exposure

Fig. 6 Profile of thermal-induced Von Mises stress on the Si-W mask structure exposed by a synchrotron source with 150 mW/cm² power density for a 1-sec exposure. (1 kgf/mm² = 9.807 × 10⁷ dyne/cm²)

Fig. 7 Temperature distribution of the Si-W mask structure after a 10 ns, $5 \times 10^8 \text{ mW/cm}^2$ plasma X-ray pulse

square pad to the region of isolated pillars. It can be seen that the higher temperatures occur at the mask areas with a greater percentage of absorber coverage. This result is very reasonable in view of the fact that more than 98% of the incoming X-ray power is absorbed by the mask regions covered with the W pattern, i.e., almost all of the X-ray flux incident on the W absorber is absorbed, whereas the uncovered regions absorb only about 33%. As shown in Fig. 5, the maximum temperature (27.13°C) occurs at the region of W square pad where the density of absorber coverage is highest.

The result of thermal stress calculations for the mask structure is shown in Fig. 6. It is observed that the thermal-induced stresses are concentrated on the Si-W interface of square pad and gratings. The calculated maximum Von Mises stress (i.e., square root of the sum of the squares of all stresses) at the Si-W interface was $1.2 \times 10^8 \text{ dyn/cm}^2$. The mismatch of thermal expansion coefficients between W absorber and Si substrate can be expected to contribute to the buildup of thermal stress at the interface region. Therefore, in this case the most probable mechanism of mask failure is the peeling of the W absorber from the Si membrane as a consequence of the induced shear stress at the interface exceeding the adhesion strength between them.

Currently X-ray mask design sometimes utilizes an intermediate layer (e.g., chromium, lead, and platinum) to provide adequate bonding between mask

Fig. 8 Time dependence of the calculated temperature on the W absorber due to a 10 ns plasma X-ray pulse

absorber and membrane. Because such intermediate layers are very thin ($200 \sim 300 \text{ \AA}$), any defect in the layers may initiate cracks and subsequent stress accumulation at the interface regions, leading to fatal denudation of the absorber from the membrane. Therefore, care is necessary in the application of such interface materials as adhesion promoters to mask design.

4.1.2 Case 2 A plot of the temperature distribution on the mask structure irradiated by a 10 ns X-ray pulse is shown in Fig. 7. It is observed that the maximum temperature of 28.25°C occurs at the W square pad, where the heat is transferred through the thickness of the W absorber. Figure 8 illustrates the

time dependence of the calculated temperature at points on the top layer and bottom layer of the W absorber. The temperature of the point on the top layer reaches a maximum at the end of the pulse (i.e., 10 ns), and then exponentially decays to a uniform temperature on a time scale of order 25 ns due to the heat conduction through the W absorber into the Si membrane. On the other hand, the temperature of the point on the bottom layer of the W absorber (near the Si-W interface) shows an increase throughout the duration of the pulse, and then stabilizes at the same temperature as the point on the top layer of the W absorber, indicating that the thermal equilibrium state is eventually reached.

Since the duration of the high-intensity pulsed X-ray irradiation is very short, especially compared to the estimated time needed for heat propagation from the mask through the helium gas to the cooled wafer (several microseconds), serious thermal impact problems can arise with the plasma source. The stress calculations of the mask structure for Case 2 shown in Fig. 9 indicate that the thermal stresses not only center on the Si-W interface, but also on the region around vias on the W square pad. The maximum calculated stress value in Case 2 was $1.6 \times 10^8 \text{ dyn/cm}^2$, which is somewhat higher than that in Case 1. It is also observed from the figure that a large stress can be induced in the vicinity of the edges (i.e., the corner points) of the W absorbers. The corner points are the locations where mask failure may take place in the

form of either excess plastic strain or absorber delamination resulting from shear loading. It is therefore reasonable to suspect that thermal cycling generated by repetitive X-ray pulses may result in unwanted mask distortion and lifetime problems. Based on the simulated results, it is suggested that it is necessary to conduct the acceleration test of thermal stress-induced mask failure for evaluating the mask thermal stability and failure threshold.

4.2 Pattern displacement contour

The calculations of temperature distributions presented above show that mask temperature rise is kept within 3.3°C by using He gas to thermally connect the mask to the wafer (i.e., mask-wafer thermal coupling). Even if the temperature is low, the thermal distortion problem may occur when a temperature gradient exists. The effect of such small temperature rise on nonlinear absorber pattern stability and overlay accuracy involved in the lithography process is still an open question.

An important and identical result obtained from the displacement analysis of the mask structure for both synchrotron and plasma source, as shown in Fig. 10, indicates that the thermoelastic displacements are directed from the center of the mask towards the mask edges. This result suggests that during X-ray exposure the in-plane distortions on the mask are not fixed but shift outward, that is, the behavior of thermal distortions is a dynamic response. In this case, the mask is expanding. It is deduce that the direction

STRESS - VON MISES MIN : 0.00374 MAX : 1.64126 (unit : kgf/mm²)

Fig. 9 Profile of thermal-induced Von Mises stress on the Si-W mask structure after a 10 ns, $5 \times 10^8 \text{ W/cm}^2$ plasma X-ray pulse ($1 \text{ kgf/mm}^2 = 9.807 \times 10^7 \text{ dyne/cm}^2$)

Fig. 10 Graphic plot of thermal displacement on the Si-W mask structure after X-ray irradiation

of the shift results from the thermal stresses acting toward the mask rims. We therefore deduce that the feature edges of the printed image on the wafer will blur due to the in-plane motion of points on the mask. This prediction is in good agreement with similar experimental results observed previously by a number of researchers.⁽⁹⁾

This thermal-induced pattern displacement, caused by the local temperature change during the lithography process, is determined by the X-ray power absorbed in the mask, the heat loss mechanism, and the elastic and geometric properties of the mask material. An estimate of the maximum displacement for the Si-W mask structure predicts a magnitude of $\delta_{\max} = 7.31 \times 10^{-8} \Delta T$ mm. In general, the absorber feature position shift must be restricted to within one-tenth of the minimum feature size (critical dimension). For quarter-micron design rule of 256 Mb DRAM, the value of $\delta_{\max}$ should be within $0.025 \mu\text{m}$. This means that the temperature change needs to be controlled to within 3.42°C . In other words, the tolerable maximum and minimum temperatures are 28.42°C and 21.58°C , respectively. Thus temperature control in the mask/wafer unit is an important issue which must be taken into account to avoid unexpected temperature variation arising from certain conditions, such as cooling system breakdown or poor cooling design.

5. Conclusion

The transient thermomechanical response of the Si-W mask structure during intense X-ray irradiation was investigated by a finite-element method. The distributions of temperature, thermal stress, and thermoelastic displacement on the mask structure were calculated for two cases using different X-ray sources: synchrotron radiation and plasma source. Although the calculation yields only approximate results, these coincide fairly well with experimental results reported by other authors. Moreover, the results should be useful and helpful for determining the optimum X-ray mask structure. Some important guidelines deduced from the simulation are summarized as follows.

(1) A more densely populated absorber pattern is expected to produce higher peak temperatures. The maximum temperature is found to occur at the W square pad which has the greatest local percentage coverage on the Si mask membrane.

(2) The thermal-induced stresses are prone to accumulate at the Si-W interface and the corners of W features. Furthermore, in the case of a plasma source, it is notable that the thermal stresses also build up in the vicinity of voids on the W square pad.

(3) During X-ray exposure, the temperature-induced pattern position shift or in plane thermal distortions are directed outward. This phenomenon indicates that the thermal stresses in the W absorber

and the Si membrane act toward the edges of the mask structure.

(4) In order to limit the thermoelastic displacement within $0.025\text{ }\mu\text{m}$ for the Si-W mask designed with a critical dimension of $0.25\text{ }\mu\text{m}$, precise control of the localized temperature variation within 3.42°C is needed.

(5) Under the conditions assumed in this study, it is confirmed that the temperature rises and corresponding thermoelastic distortions on the mask can be accommodated within the acceptable limits when using helium as a heat exchange medium which has a high thermal conductivity and absorbs little X-ray flux.

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