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Modeling Spectral Absorptance of Silicon Wafers

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Abstract. This paper presents a parametric study of the radiative properties of silicon patterned wafers, considering the effect of wavelength, and polarization. The finite-difference time-domain (FDTD) method is employed to examine the effect of various trench and gate sizes on the spectral absorptance via numerically solving the Maxwell's equations. The effective medium theory (EMT) is also used to help explain the absorptance prediction. In the cases with trench size variation, clear interference effects were shown at long wavelengths for the TE wave, but the multiple reflection effect starts at a much shorter wavelength for the TM wave. In the cases with polysilicon gate variation, while the gate sizes are very small compared to wavelength, the results show rather unusual phenomena. The absorptance calculated by EMT is in agreement with FDTD in the cases with small gate and period sizes. With the increase of period and decrease of the ratio of the gate width to the grating period, both EMT and FDTD results for the TM (transverse magnetic) mode approach to pure silicon since the grating effect diminishes. The effects of the diffraction, wave interferences on the spectral absorptance were also discussed. This work is of great importance for optimization of advanced annealing techniques in semiconductor manufacturing.

Keywords: finite-difference time-domain method, effective medium theory, radiative property, periodic nanostructure, patterned wafer

1. Introduction

According to the International Technology Roadmap for Semiconductors [1], the gate length and junction depth of the 65-nm devices used in high-performance complementary metal oxide semiconductor (CMOS) technology will be 25 and 13.8 nm, respectively. Rapid thermal processing (RTP) currently provides the high-temperature annealing needed to create ultra-shallow junctions. However, conventional RTP tools that use tungsten-halogen lamps for heating encounter a dilemma between limiting the junction depth and maximizing the degree of electrical activation of implanted dopants. The ion implantation annealing time, which ranges from 1 to 10 s above 1000℃ in the conventional RTP, is too long to confine ion diffusion and achieve the implanted doping distribution within the junction [2]. This difficulty can be overcome by using high-intensity flash-lamp or laser annealing with heating pulses lasting only a few miliseconds. The typical energy sources are Ar or Xe arc lamps, which mainly emit ultraviolet and visible radiation. In flash-lamp heating, optical energy is absorbed on the wafer front side because of the small penetration depth that results from the large absorption coefficient of Si within the lamp spectrum. Because the energy is absorbed within milliseconds, thermal diffusion cannot distribute heat uniformly across the wafer surface. Therefore, temperature uniformity across the wafer surface continues to be a critical issue even with the new annealing processes. Temperature nonuniformity may cause uneven activation of the implants, as well as excessive thermal stress that can introduce crystallographic defects [3-5]. One major reason for the temperature nonuniformity arises from the difference in the absorptance of various device patterns in different regions of the wafer surface. Many researchers have modeled the radiative properties of different patterned structures on wafers and obtained reasonable agreement with experimental results. However, earlier investigations explored the behavior for relatively simple patterns with features on the order of micrometers and at

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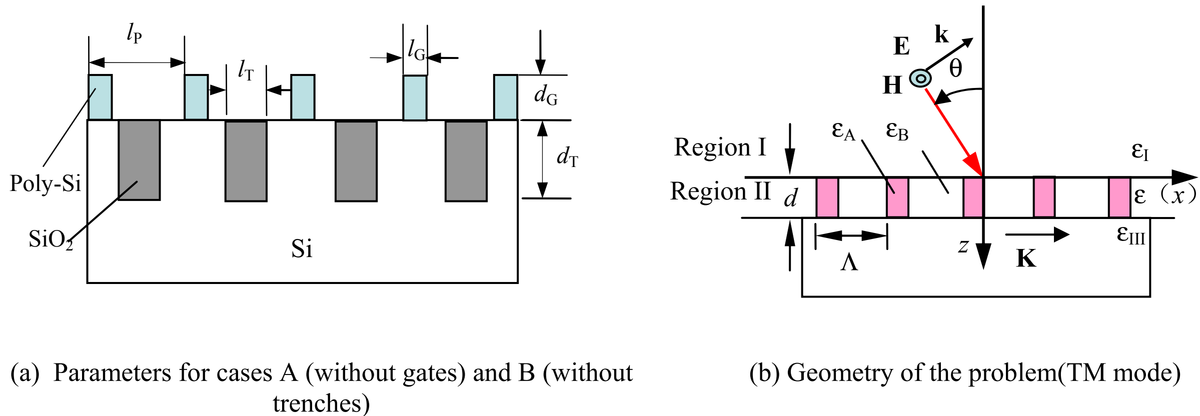
wavelength longer than 0.4 μm, i.e. ultraviolet wavelengths were not considered [6]. Radiative properties of nanostructures may be very different from those of microstructures made of similar materials. It is essential to know the spectral absorptance of the patterned wafers across a broad range of wavelengths, including the ultraviolet region, so the amount of energy absorbed from the flash-lamp can be determined accurately. Little is known about the influence of nanoscale patterns on the radiation absorption and reflection during the millisecond annealing process. The objective of this paper is to model the radiative properties of periodically patterned wafers with nanoscale linewidth. The effects of wafer sizes, wavelength, and polarization on the spectral absorptance are investigated for the selected two-dimensional (2D) patterned structures with multilayer gratings. In the present study, the finite-difference time-domain (FDTD) is employed to numerically solve the Maxwell's equations and obtain the radiative properties of various wafers front side geometries. Previous studies have used the effective medium theory (EMT), in which the grating region is treated as a homogeneous layer with an effective dielectric function. EMT is often helpful for understanding the behavior of sub-wavelength gratings with small period-to-wavelength ratios.

In this study, the structures considered are SiO2 trenches embedded in the Si wafer, and polysilicon gate arrays on the Si substrate. The wavelength range of the radiation from the heat source is from 200 to 1000 nm. The incident radiation is at normal angle of incidence with the plane of incidence perpendicular to the gratings. Extensive feature size variations, in conjunction with the wavelength variations, were considered for different nanostructures on the wafer front side. The effect of diffraction, wave interference on the spectral absorptance was discussed.

2. Model Structure Analysis

Fig.1(a) illustrates a Si wafer that includes trenches filled with SiO_2. Fig.1(b) depicts a polysilicon gate array on the Si substrate. Fig.1(c) gives important parameters needed in the analysis of the absorptance of the patterned wafer, upon which the electromagnetic wave irradiates. Region I is free space with $\varepsilon_I = n_I = 1$ and $\kappa_I = 0$, where $\varepsilon = (n + i\kappa)^2$ is the dielectric function. Region II is composed of material A and material B such that its dielectric function is a period function of x with a period Λ, which is the grating period. Region III is the substrate with a dielectric function, ε_{III}. For simplicity, it is assumed that incidence wave vector is on the x-z plane, that is, the y component of k is zero. For a transverse magnetic (TM) wave, the magnetic field H is perpendicular to the plane of incidence, i.e. parallel to the y direction and perpendicular to the grating vector K, as shown in Fig.1(c). On the other hand, for a transverse electric (TE) wave, the electric field E is perpendicular to the plane of incidence and the vector K. The dimensions of the structures examined in this study are listed in Table 1. This study assumes that the structures are 1D gratings, the depth of the trenches is fixed at d_T=300 nm and gate height is fixed at d_G =100 nm. The structures of group A help us understand the consequences of variations in the density of patterns on wafers, as reflected in the ratio of the pattern. The structures of group B help us explore the effect of the varying ratio of gate width (silicon bars) to the pattern pitch for the fixed gate width.



(a) Parameters for cases A (without gates) and B (without trenches)

(b) Geometry of the problem(TM mode)

Fig. 1: Illustrations of the device and model structures.

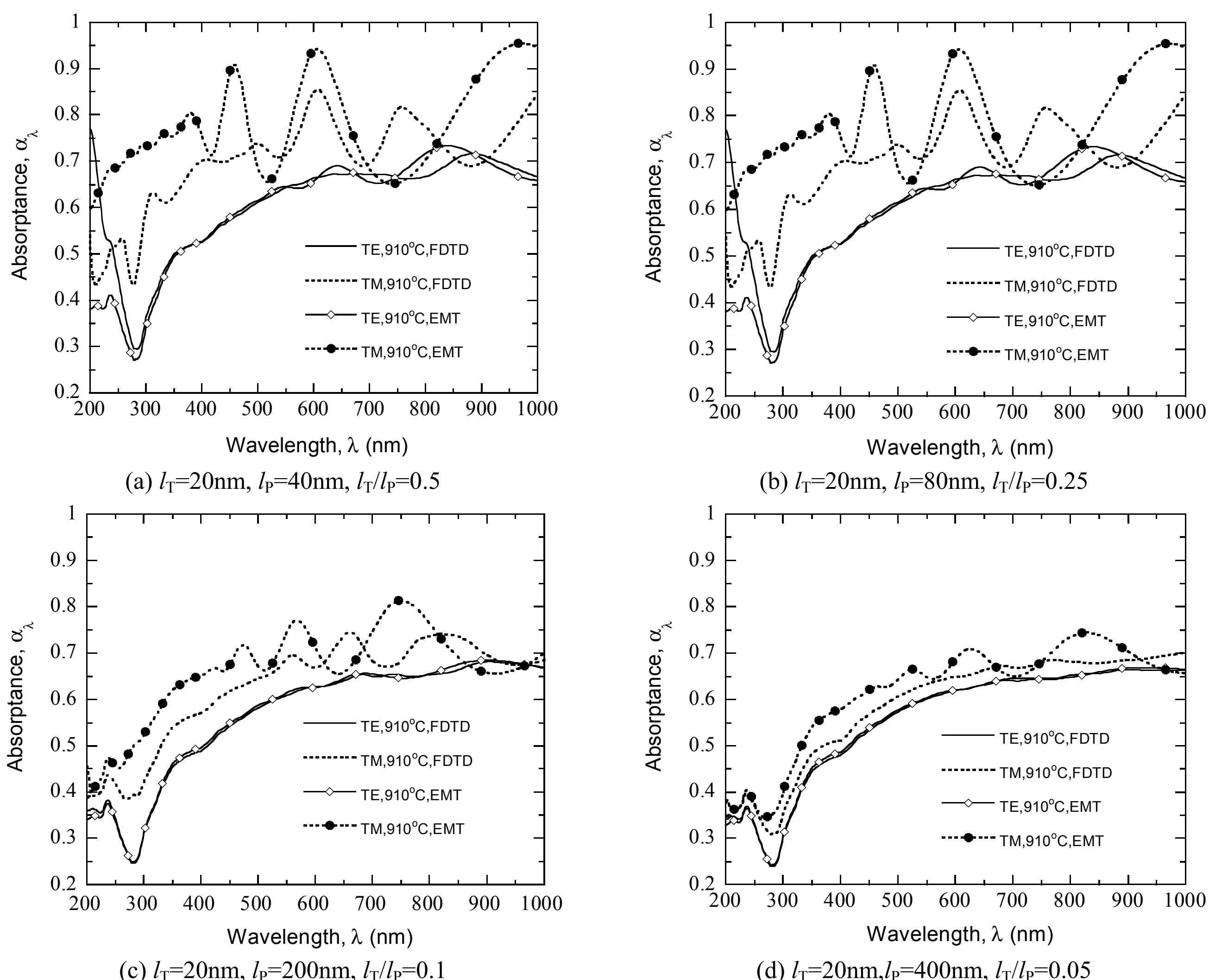
Table 1 Geometry of the studied structures

A	l_T	L_P	l_T/l_P	B	l_G	l_P	l_G/l_P
1	20	40	0.50	1	30	60	0.50
2	20	80	0.25	2	30	120	0.25
3	20	200	0.10	3	30	300	0.10
4	20	400	0.05	4	30	600	0.05

3. Results and Discussion

3.1. Trench structures in the a group

Fig. 2(a) shows clear interference effects at long wavelengths. For the TE wave, the interference appears at wavelength longer than 540 nm. According to thin film theory, interference happens when the extinction coefficient is small enough, or $\kappa\delta_T/\lambda$ is small enough,. Note that the multiple reflection effect starts at a much shorter wavelength for the TM wave. Fig.2 also shows that the EMT prediction improves when the l_T/l_P ratio is small except at small wavelength. It is of course true when the ratio is close to 1. However, EMT does not agree with FDTD result for the TM wave at short wavelength, as shown in Fig. 2(a), and the absorptance of the TM wave from EMT in Fig. 2(d) clearly shows oscillations that are not predicted by the FDTD method. For the short wavelength in Fig. 2(a), the EM wave could be treated as ray tracing energy bundles which separate the reflection from Si and that from SiO_2 trench, instead of the diffractive wave which is not significant at short wavelengths.



(a) l_T=20nm, l_P=40nm, l_T/l_P=0.5

(b) l_T=20nm, l_P=80nm, l_T/l_P=0.25

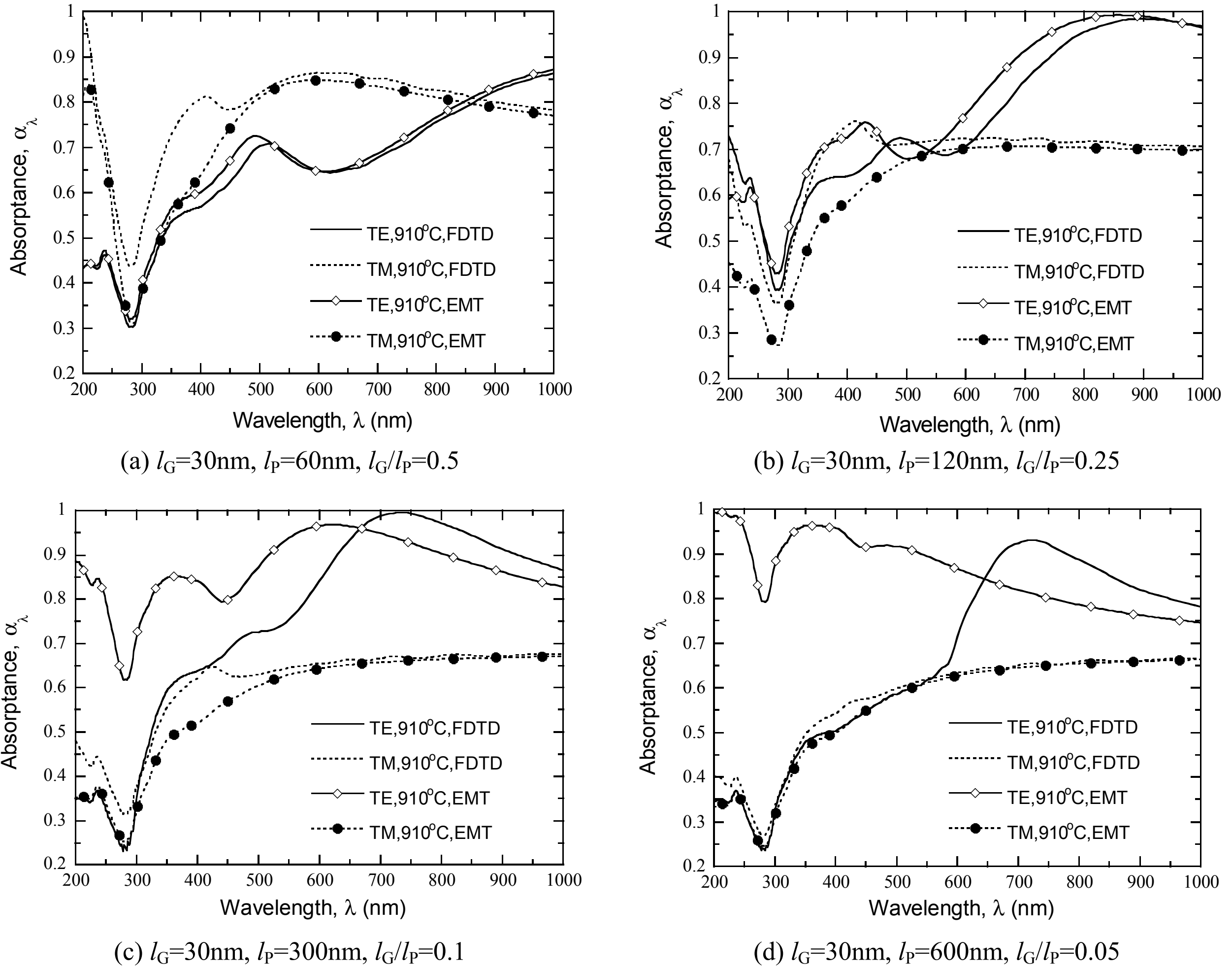
(c) l_T=20nm, l_P=200nm, l_T/l_P=0.1

(d) l_T=20nm,l_P=400nm, l_T/l_P=0.05

Fig.2: Absorptance spectra for A cases at θ= 0°.

3.2. Polysilicon gate structures in b group.

Fig.3 (a) shows that the absorptance calculated by EMT is in agreement with FDTD except for some small difference at short wavelengths. The agreement is expected due to the small gate and period sizes. Even though the penetration depth might be smaller than the gate height 100 nm at small wavelength, it is comparable to the gate size, and the neighboring medium of the gate is air, which makes it easy for incident light to be diffracted into the space between gates. This tends to reduce the error of EMT. Fig.3 (b) shows the absorptance with smaller l_G/l_P and larger l_P. While the EMT results still give a good agreement, the error at short wavelengths increases. With the increase of period and decrease of l_G/l_P ratio, both the EMT and FDTD results for the TM mode approach to pure silicon since the grating effect diminishes. However, the error of the EMT results for the TE mode becomes considerable, as shown in Fig.3(c) and 3(d). The error is caused by the limitation of EMT, which requires the period to be significantly smaller than the wavelength.



(a) l_G=30nm, l_P=60nm, l_G/l_P=0.5

(b) l_G=30nm, l_P=120nm, l_G/l_P=0.25

(c) l_G=30nm, l_P=300nm, l_G/l_P=0.1

(d) l_G=30nm, l_P=600nm, l_G/l_P=0.05

Fig.3: Spectral absorptance for B cases at normal incidence.

To understand how the gate height influences the overall grating TE absorptance, several gate heights are selected: 20 nm, 40 nm, 60 nm, and 80 nm. In the Fig.4, when gate height is 20 nm, the absorptance curve is close to that of pure silicon. However, when the height increases to 40 nm or above, the gate height significantly changes the absorptance curve. This shows that a slight increase in the gate height can drastically increase the absorptance or produce the equivalent effect of anti-reflection coating. The increased gate height shifts the peak absorptance to longer wavelength due to the increase of optical path length in effective thin film.

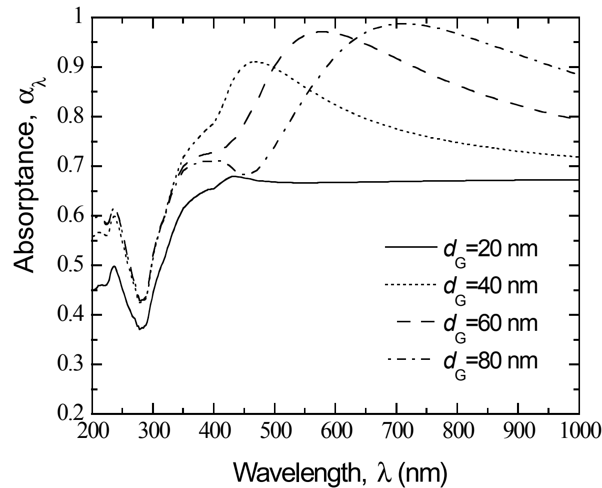


Fig.4: The TE wave absorptance for B-2 base case at normal incidence with different gate heights.

4. Summary

An extensive numerical study of the absorptance of the patterned wafer is presented. The wavelength range of interest, 200-1000nm, covers the radiation heat sources of flash-lamp arc. The finite-difference time-domain method and the effective medium theory are used to solve the electromagnetic wave propagation in nanoscale device structures.

(1) It is found that at small filling ratio and small periods (sub-wavelength gratings) the effective medium theory can describe the spectral variation reasonably well, especially for the TE wave.

(2) As for the SiO_2 trenches embedded in the silicon wafers, clear interference effects were shown at long wavelengths for the TE wave, but the multiple reflection effect starts at a much shorter wavelength for the TM wave. The EMT prediction improves when the l_T/l_P ratio is small except at small wavelength, especially for the TE wave.

(3) When the gate height increases from 20 nm to 40 nm or above, the gate height significantly changes the absorptance curve. The increased gate height shifts the peak absorptance to longer wavelength.

(4) This study improves the understanding of the geometrical effects of device features on the radiative properties, which is important for optimization of advanced annealing techniques in semiconductor manufacturing.

5. References

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