The Effect of the Fractal Clusters on the Si (111)-7×7 Surface

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Abstract: one of the most important ingredients responsible for the success of integrated silicon technology is the Metal Oxide Semiconductor Field-Effect Transistor (MOSFET), and a major reason for its success is the MOSFET's scalability. Although the industry uses silicon and silicon dioxide in the electronic devices, it can be used for opto-electronic devices as well due to formation of fractal oxide clusters on the silicon substrate. The Nano-opto electronics revolution has been possible through an extensive study of the optical properties of silicon dioxide structure on silicon substrate. This includes an investigation of the surface structure and stacking fault of silicon and oxygen atoms on Si (111)-7×7 surfaces. Indeed, there are some issues which are playing important rules in the formation of the long-wavelength absorption spectral wing. One issue is stacking fault atoms in the Si (111)-7×7 unit cell which determines the monotonic decrease of absorption with increase of wavelength and the other issue is due to incoming oxygen atom which leads to breaking silicon and oxygen bonds and causes the appearance of the additional spectral maximum. We have thus studied the effect of variation of the parameters of fractal clusters on optical spectra by using coupled-dipole method. In this work, we considered particle electrodynamics dipole-dipole interactions, for the appearance of individual specific features in the spectral absorption.

Key words: Thin film . silicon dioxide . Si (111) . nanoaggregates . optical extinction spectra . nano transistor . MOSFET and dipole polarizability

INTRODUCTION

The Field-Effect Transistor (FET) has turned out to be the most valuable conventional electronic device. For this purpose we have tried to study the substrate and gate dielectric structure to understand the promise of nano-opto electronic applications. Silicon is a key element of the all electronics such as computer processors and memory chips because of abounding of this material in nature and forming the best oxide with oxygen molecules and oxygen atoms. It can be utilized for a large number of different applications, from electronic devices to opto electronic devices which has led to an enormous development in the electronics and nano-electronic industry [1-9] despite of its substantial standby and leakage power which causes high power consumption of strongly scaled devices.

Many researchers have grown silicon dioxide on silicon substrate and studied extensively it's structure by many using several different techniques such as XPS [1], polarization-and photon-energy-dependent UPS [10], x-ray-induced Auger spectroscopy [4-6] and STM [11, 12]. Several proposals based on both measurements and theoretical calculations have been given in the literature on the initial reaction between oxygen and the silicon surface. At low oxygen exposure a metastable state is formed. Both a molecular and an atomic model for this state have been proposed. One suggestion is that this corresponds to an oxygen molecule forming a bridge between two silicon atoms or interacting with a single adatom. Another suggestion for the metastable state is an atomic model where the oxygen molecule dissociates and the oxygen atoms go into the adatom back-bonds or dangling bonds [8].

In this work, we considered particle electrodynamics dipole-dipole interactions and found the frequency dependence of the permittivity of this material using symmetry with respect to rotations and the averaging over the entire aggregate orientations. This is because particle aggregation is accompanied by the formation of fractal structures, which are assembled from the main portion of the initially oxidation while oxygen atom inserted into silicon.

EXPERIMENTAL DETAILS AND RESULTS

The silicon samples (n-type, 5Ω cm, 3 cm×1 cm) were polished from one side to ensure a smooth surface and cut out of wafers. We rinsed them with ethanol and put them in an ultrasonic bath for one hour. The cleaned

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samples may be oxidized with oxygen molecules in the media or make bonds with carbon atoms, we cleaned them one more by passing current through the samples several times and every time we got spectra to be sure that the samples are clean. The initial oxide growth was done in the ultrahigh vacuum (UHV) chamber. The chamber was then baked before the experiments. After baking the background pressure was 2×10^{-10} Torr.

Earlier, measurements with a residual gas mass spectrometer in the line of the beam, has shown that a very high proportion (about 50 per cent) of oxygen is produced with this setup. Typical total pressures in the chamber during exposure of oxygen into the vacuum chamber were around 5×10^{-7} Torr. Indeed, we do not need to consider several STM (Scanning Tunneling Microscopy) spectra, because the initial oxide growth on the Si (111)-7 × 7 surface is demonstrated in Fig. 1.

The images were measured with a bias voltage of 3. As one can see the initial oxide growth is cluster form and the ultra thin oxide film is fractal film. We tried to show this image to be sure that the islands can affect the optical properties of oxide film.

This problem provides information about the most practically important physical characteristics of islands. The image shows the changes of the electronic structure or the morphology of small islands when a transition from the silicon substrate to clusters occurs.

These regularities can produce the dramatic changes in color of radiated ray or light like the origin of the intense color of sols containing small noble metal particles as Karpov and coworkers explained in details [13]. Based on their idea the optical properties of the fractal clusters can be used for describing the evolution of optical spectra of silicon with incoming oxygen molecules or atoms within the range of most characteristic occupied site sizes (5-30 nm).
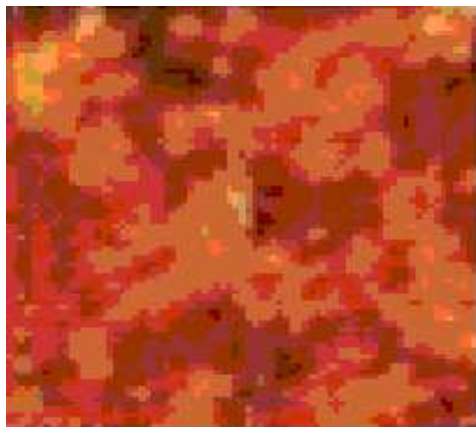

Fig. 1: STM image of the oxidized Si(111) 7×7 surface for 20 seconds acquired over an area of 500°A by 500°A and with a bias voltage of 3 V

COAGULATION OF OXYGEN ATOMS AS FRACTAL FILM ON SILICON SUBSTRATE

Over recent decades, a remarkable progress has been made in the development of theoretical models of optical absorption by the aggregated oxygen atoms on the silicon surfaces. Many people have applied the method of coupled dipoles to the colloid metal sol aggregates [13 and references therein]. The most widespread viewpoint about the changes of the electronic structure of small particles during transition from the bulk materials to clusters and the variations of its color, beginning with the well-known work by Mie [14]. Mie and coworkers considered the spectral selectivity of scattering and absorption, which is governed by the particle size. They believed that variations of the optical spectra of noble metal colloids are due to different size of these noble metal particles. It means that the position of maximum of absorption (scattering) band (λ_r) depends on particle size, and causes the appearance of the long-wavelength wing in the absorption spectrum.

As mentioned, there are no metal sols and we thus cannot use the Mie theory, but the clusters size may effect the broadening of the absorption spectra.

If we consider that λ_r as the wavelength of the surface plasmon, we then expect that λ_r depends on the clusters size which could be shown on average by L. By looking at Fig. 1, it is clear that clusters is accompanied by the formation of fractal structures, which are assembled from the main portion of the initially-isolated small islands. Moreover, the nearest neighbor's islands influences can be the strongest respect to the other island which is far away. This may obviously lead to a noticeable shift in the frequency of the intrinsic optical resonance of particles (ω_r). As our theoretical investigations in the next section will show, the reason for such a this shift of frequency is due to the dipole-dipole interactions between the incoming oxygen-induced (oscillating) dipole moments and the atoms of the neighbor's cluster atoms. The traveling waves cannot transmit because of fractal objects where could not keep its translational invariance case.

Therefore, we have to find a new approach to describe optical properties of clusters. The suitable theory for this purpose is the theory of optical properties of fractal clusters (OPFC) [15-17] which give us the unique correlation between the structural and optical properties of fractal islands.

DIPOLE POLARIZABILITY OF A SINGLE OXIDE CLUSTER

We pointed that the dipole-dipole interactions are responsible color changes and coagulation of atoms.

in this case, their intrinsic kinetic energy is transformed into the kinetic energy of translational and rotational motion of an aggregate. For about N of the clusters formed with dipole-dipole interactions, the fractal structure of typical cluster located at point $\mathbf{r_i}$ will be polarized by the other cluster filed called external field $E_i^{(0)}$. From [16] the dipole moments, d, induced on different clusters obey the system of below equations

$$d_{iX} = d^{(0)} - d^{ij} \qquad (1)$$

Where

$$d_{iX} = d^{(0)} - d^{ij} \qquad (2)$$

and

$$d^{ij} = \chi_0 \sum_Y \sum_{j=1, j\neq i}^N \frac{\delta_{XY} - 3n_X^{ij} n_Y^{ij}}{r_{ij}^3} d_{jY} \qquad (3)$$

In this equation i, j = 1, 2, 3, …, N, X, Y = {x, y, z}, χ_0 is the dipole polarizability of a single cluster, $r_{ij} = r_i - r_j$ and $n = r_{ij}/ r_{ij}$. For the smooth growth oxide film in the small island, there is smooth oxide film $E_i(0)$ of ith cluster can be considered as uniform and independent of i. As Karpov and coworkers suggested, the dipole moment which induced on the ith cluster can be expressed via the corresponding linear polarizability, $\chi_{XY}(i)$ as

$$d_{iX} = \sum_Y \chi_{XY}^{(i)} E_Y^{(0)} \qquad (4)$$

The second term in the right side of the Eq. (2) is a matrix. It is clear that this matrix is symmetrical and can be reduced to the diagonal form via an orthogonal transformation in the 3N-dimensional space of the vectors d and $E^{(0)}$ with components d_{iX} and $E_{iX}^{(0)}$ so that

$$\langle i X | M | j Y \rangle = \frac{\delta_{XY} - 3n_X^{ij} n_Y^{ij}}{r_{ij}^3}$$

$$i \neq j, \langle i X | M | j Y \rangle = 0$$

It yields to

$$d^{ij} = \chi_0 \sum_Y \sum_{j=1, j\neq i}^N \langle i X | M | j Y \rangle d_{jY}$$

and

$$\frac{d^{(0)}}{\chi_0} = E_{iX}^{(0)}$$

$$\frac{d^{ij}}{\chi_0} = E_{XY}^{(ij)}$$

Then

$$E_{XY}^{ij} = \sum_Y \sum_{j=1, j\neq i}^N \langle iX | M | j Y \rangle d_{jY}$$

$$\Rightarrow E = Md$$

Where

M =

$$\begin{pmatrix} I_{11}^* & 0 & 0 & \dots \\ 0 & I_{22}^* & o & \dots \\ 0 & 0 & I_{33}^* & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \begin{pmatrix} M_{11} & 0 & 0 & \dots \\ 0 & M_{22} & o & \dots \\ 0 & 0 & M_{33} & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \begin{pmatrix} I_{11} & 0 & 0 & \dots \\ 0 & I_{22} & o & \dots \\ 0 & 0 & I_{33} & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \qquad (5)$$

By introducing the particle's (or atom's) resonance frequency, f, and relaxation rate (γ), we can write$-1/\chi_0$ into real and imaginary parts in which imaginary part, Im χ_0 give us the absorption spectrum of the fractal aggregate. Therefore,

$$\frac{1}{\chi} = -\frac{\hbar}{|d^{ij}|^2} \begin{pmatrix} f_{11} + i\gamma_{11} & 0 & 0 & \dots \\ 0 & f_{22} + i\gamma_{22} & 0 & \dots \\ 0 & 0 & f_{33} + i\gamma_{33} & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \qquad (6)$$

The summation of Eq. (5) and Eq. (6) leads to a matrix, H, in that

$$d = \frac{1}{|H|}$$

$$\begin{pmatrix} I_{11}^* & 0 & 0 & \dots \\ 0 & I_{22}^* & o & \dots \\ 0 & 0 & I_{33}^* & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \begin{pmatrix} H_{11} & 0 & 0 & \dots \\ 0 & H_{22} & o & \dots \\ 0 & 0 & H_{33} & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \begin{pmatrix} I_{11} & 0 & 0 & \dots \\ 0 & I_{22} & o & \dots \\ 0 & 0 & I_{33} & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} E \qquad (7)$$

We introduce $I_{a(\beta)}$ as $I_{\beta(a)}$ transpose matrix

$$d = I_\alpha H^{-1} I_\beta E^{(0)} \qquad (8)$$

or

$$d_{iX} = \sum_Y \sum_{j=1}^N \sum_{n=1}^{3N} I_{iX}^n I_{iY}^n H_n^{-1} E_{jY}^{(0)} \qquad (9)$$

Comparing Eq. (4) and Eq. (9), the linear polarizability, $\chi_{XY}^{(i)}$ is :

$$\chi_{XY}^{(i)} = \sum_{j=1}^N \sum_{n=1}^{3N} I_{iX}^n I_{iY}^n H_n^{-1} \qquad (10)$$

I_{iX}^n and H_n^{-1} are the eigenvalues of the vector and matrix M, respectively. As pointed before, the linear polarizability, $\chi_{XY}^{(i)}$ of the particle in average averaged over the particle number N which is equal to 1/N what we obtained in Eq. (10), i.e.;

$$\chi = \frac{1}{3} \sum_X \chi_{XX} = \frac{1}{3N} \sum_X \sum_{j=1}^N \sum_{n=1}^{3N} I_{iX}^n I_{iX}^n H_n^{-1} \qquad (11)$$

or

$$\chi = \frac{1}{3N} \times \frac{1}{|H|}$$

$$\begin{pmatrix} I_{11}^* & 0 & 0 & ... \\ 0 & I_{22}^* & o & ... \\ 0 & 0 & I_{33}^* & ... \\ ... & ... & ... & ... \end{pmatrix} \begin{pmatrix} H_{11} & 0 & 0 & ... \\ 0 & H_{22} & o & ... \\ 0 & 0 & H_{33} & ... \\ ... & ... & ... & ... \end{pmatrix} \begin{pmatrix} I_{11} & 0 & 0 & ... \\ 0 & I_{22} & o & ... \\ 0 & 0 & I_{33} & ... \\ ... & ... & ... & ... \end{pmatrix}$$

But the imaginary part should be obtained for analyzing the absorption spectrum of the fractal structure of any cluster. By considering the relaxation rate and resonance frequency as ω_r we have:

$$Im\chi = \frac{1}{3N} \sum_X \sum_{i=1}^N \sum_{j=1}^N \sum_{n=1}^{3N} I_{iX}^n I_{iX}^n \times \frac{\hbar\gamma}{(-\hbar\omega_r + d_{XX}M_n)^2 + \hbar^2\gamma^2} \quad (12)$$

There are ω_r and γ in Eq. (12) which indicate that the dipole polarizability of a cluster depends on resonance frequency and relaxation rate. The relaxation rate is related to homogeneous half width which means the polarizability can be changed with surface plasmon and many other phenomena in the spectrum.

CONCLUSION

The initial silicon atom reactions occurring just after the exposure oxygen and the oxide clusters are formed on Si(111)-7 × 7 as shown STM image. This indicates different states on the surface. We believe that the nearest neighbor clusters can strongly affect to each other. Indeed, distance between geometrical centers (we assume a point at L/2 inside each cluster as a center of correspond cluster) of the nearest atoms inside the clusters is the crucial importance for the OPFC theory. The main reason for the significant broadening of the absorption spectra of typical film which has been shown with researchers (refer to [13] and references therein), is the assembling of atoms of the dispersed phase into fractal clusters. In conclusion, we found that a clear and strong correlation between the optical properties of the ultra thin oxide film and the cluster structure. This phenomenon causes the variation of polarizability of the ultra thin film and the optical properties of the clusters. From the relationship between frequency and wavelength and Eq. (12) based on OPFC theory, we found that the aggregation of oxygen atoms into fractal structure of cluster gives rise to a giant broadening of the long-wavelength wing of the absorption spectra which may become commensurable with the magnitude of the resonance frequency itself.

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