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Full 3D Monte Carlo simulation of pit-type defect evolution during extreme ultraviolet lithography multilayer deposition

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ABSTRACT

To model key aspects of surface morphology evolution and to overcome one of the main barriers to the implementation of extreme ultraviolet lithography in semiconductor processing, the 3D Monte Carlo simulation of ion-beam deposition on pit-type defects was performed. Typical pit defects have depths in the 5–20 nm range and are about 10 times that wide. The aspect ratio of a defect cross section defined as depth divided by the full width at half maximum was used to measure the defect profile (decoration) as a function of film thickness. Previous attempts to model this system used 2D level set methods; 3D calculations using these methods were found to be too computationally intensive. In an effort to model the system in 3D the simulation of this study used the Solid-on-Solid aggregation model to deposit particles onto initial substrate defects. Surface diffusion was then simulated to relax the defect. Aspect ratio decay data was collected from the simulated defects and analyzed. The model was validated for defect evolution by comparing simulations to the experimental scanning transmission electron microscopy data. The statistics of effective activation energy were considered to show that observed defects have important geometric differences which define a unique aspect ratio decay path. Close fitting to the observed case was utilized to validate Monte Carlo physical models of thin film growth for use in predicting the multilayer profile of pit-type defects.

1. Introduction

This is an inquiry into the time evolution of localized negative space in a thin film undergoing energetic deposition. Understanding and being able to control the evolution of significant negative space could have important applications in nano-scale materials fabrication [1]. There has been much work done on the characterization and mechanism of nanostructure formation during surface growth. In general the use of lattice Monte Carlo simulations to probe the morphology and scaling properties of film growth is well established in the literature [2–7]. However, little-to-no similar work has been done on the time evolution of localized pits and negative space, despite work done on other localized phenomena such as fanning from point seeds [8]. In this initial work the goal is to validate Monte Carlo simulations of thin film growth for use in modeling the morphology evolution of low aspect ratio pit defects as seen on mask substrates used in extreme ultraviolet lithography (EUV).

EUV lithography is a next-generation lithography technology which is poised to replace Deep Ultraviolet Lithography in the fabrication of smaller semiconductor devices as the industry tries to keep up with Moore's law [9,10]. EUV uses an exposure wavelength of 13.5 nm, which is absorbed by most materials, hence all the optical components need to be reflective. This places very tight requirements on EUV photomasks to meet roughness, flatness and defectivity specifications [10], and one of the major problems preventing the commercial implementation of EUV lithography is the production of defect free mask blanks [9].

EUV masks are Bragg reflectors whose fabrication requires tight morphology control in order to operate at the 13–15 nm wavelength range [11]. The optical coatings consist of 40–50 Mo/Si bilayers of 3 nm and 4 nm, respectively. The interface widths between layers are less than 1 nm [12]. In the past EUV multilayers have been grown using e-beam evaporation [13] and magnetron sputtering [14], but ion-beam deposition is used currently mainly because of low particle adders during deposition. Ion beam deposition helps to smooth the upward growth because more energy is delivered to the surface than many other deposition methods, enhancing diffusion [11].

Initial defects on the substrate lead to EUV mask defects after the aggregation of the multilayer. The EUV mask defects distort the indented multilayer geometry causing destructive optical behavior [12]. Initial substrate defects can be either a particle or a pit on the surface [15]. As the defect size decreases below 70 nm size, there is an exponential increase in the number of defects present on the substrate and a majority of these are pit-type defects [16]. These defects are caused mainly by the chemical mechanical polishing and cleaning processes, which are needed to produce the required sub-Angstrom surface roughness. Moreover, pit-type defects are an unavoidable problem, because removing embedded particle defects leaves a pit-type defect in their

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place [17]. There have been experimental approaches to smooth pit-type defects using the ion-beam deposition system—but they suffer either from high defectivity [18], or are limited by the narrow process window required to keep the specifications of ML reflectivity and uniformity within range [19].

Hence, for the purposes of this exploration only the time evolution of pit-type defects are considered. This situation is well-suited to study the evolution of negative space due to the high attention paid to creating abrupt and smooth interfaces between bilayers. This allows for good measurements of the aspect ratio evolution. A Scanning Transmission Electron Microscopy (STEM) cross section of the observed physical behavior is shown in Fig. 1.

The surface relaxation observed during the aggregation of this optical coating presents a fundamental battle between surface geometry and the bombardment of noise from deposition. Through the process of diffusion the geometric information of the initial defect is eroded into flatness. Any process by which the morphology of a surface is smoothed is driven by this battle. Any arbitrary surface morphology can be thought of as being composed of many pits, of differing size scales. Studying one localized example of defect decay contributes to a more fundamental understanding of the smoothing process.

The EUV community has come to realize the near-impossibility of obtaining zero-defect mask blanks and considerable efforts have been directed at defect mitigation by locally modifying the absorber pattern in order to render the defects unprintable [20]. In order to predict (and correct) how the defects affect the local pattern it is essential to correctly simulate how the light interacts with the multilayers over the defect, and for this it is essential to know the multilayer growth profile over the defect.

Accurately predicting the multilayer structure would enable better optical simulations of defect printability and mitigation. There has been work on modeling the nucleation and growth of defects which are initial particles on the substrate [12]. There has been no academic work on predicting the time evolution of pit-type defects. The only known work was by the semiconductor research consortium SEMATECH who used level set methods [21] to propagate the initial surface structure through time [22]. This level set modeling as used today has several shortcomings, one being that the calculations are performed on a 2D cross section only. A full 3D calculation would be too computationally intensive. Another limitation being that the particle flux is constant and from a particular direction, while in physical deposition conditions there can be a flux distribution [22]. Performing a full 3D Monte Carlo simulation enables more realistic flux distributions to be tested if needed. Dynamics of the system such as swinging the substrate or changing the deposition angle as a function of film thickness can also be tested in order to optimize filling.

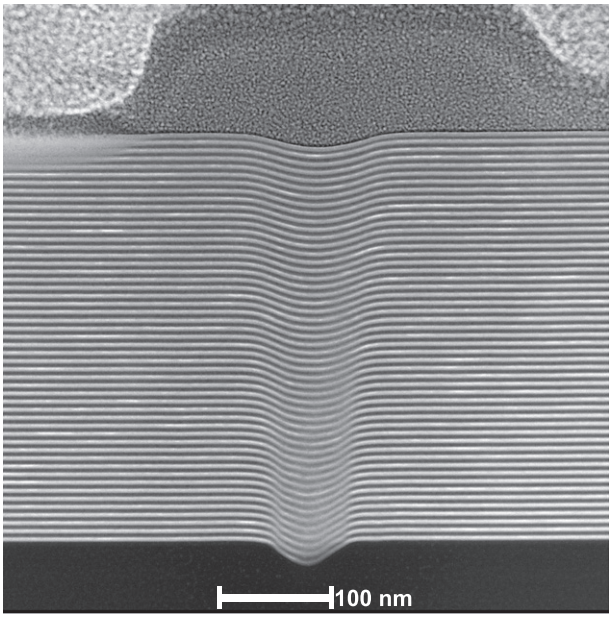

Fig. 1. A Scanning Transmission Electron Microscopy image of a defect cross section which has undergone ion-beam deposition to add 50 Mo/Si bilayers of 3 nm and 4 nm, respectively. The simulations are seeking to model the multilayer morphology evolution as measured by aspect ratio.

Characterizing the negative space with some observable, which can be obtained both from experimental data such as Atomic Force Microscopy (AFM) or STEM, and from computational data and then exploring the behavior as a function of film thickness is the basis for comparison of defect decay. For the purposes of this study the observable is aspect ratio, AR, defined as depth, d divided by the full width at half maximum (FWHM) giving a decay as the defect is filled. The variable being used in place of time is the film thickness denoted as h. The universal behaviors of defect evolution which arise from this complex system of particles can be reproduced by the simplified physical modeling of dominating behaviors which shape the growth. The two dominating behaviors for this system being the stochastic aggregation of particles and surface diffusion.

Monte Carlo simulation via the ballistic aggregation of seeds in $2 + 1$ dimensions keeps full 3D track of all particles in the aggregate. In order to model this smooth upward growth of bilayers, the Solid-on-Solid approximation to the ballistic aggregation model is used. Only the heights of the top of the surface are stored. Modeling this smooth growth using ballistic aggregation would require many more possible diffusion events, slowing execution considerably. Constraining the surface to the Solid-on-Solid model produces the roughness of the multilayer well. In the low pressures under which common deposition techniques are performed the mean free path of a particle is usually significantly larger than the distance it must travel to the substrate [23]. This allows the simulation to assume that particles follow straight lines.

2. Simulations

A Solid-on-Solid simulation of thin film deposition is conceptually simple. The surface is represented as a two dimensional matrix of heights. The initial height matrix is called a simulation template. A particle is spawned at a randomly selected lattice point at the top of the simulation. It is then propagated according to the chosen velocity distribution. Deposition direction, velocity distributions, and substrate dynamics all change how the particle is propagated to the surface. If the particle hits the aggregate it can be deposited or reemitted depending upon the sticking coefficient. After a particle is deposited there are many chances for diffusion events to occur which are all governed by the diffusion probability shown in Eq. (1) [2,24,25]

$$exp[-(E_a + n_n E_n)/kT], \tag{1}$$

where E_a is the activation energy for diffusion, n_n is the number of nearest neighbors, and E_n is the bonding energy with a nearest neighbor. A diffusing particle is chosen randomly from the surface atoms. Diffusion schemes using a window of possible particles to diffuse located around the last deposited particle were explored and found, for this phenomenon, to not produce any discernible difference. The temperature of the system is denoted as T with the Boltzmann constant as k. The quantity $E_a + n_n E_n$ can be thought of as an effective activation energy for a surface diffusion event, this quantity is denoted as E_A and is an important consideration because this value encodes differing probabilities of diffusion based upon local geometric considerations.

For each deposited particle there are many possible diffusion events, this is because of the difference in time scale of surface diffusion events compared to deposition events. For this study there are