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Extraction of roughness parameters at nanometer scale by Monte Carlo simulation of Critical Dimension Scanning Electron Microscopy

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ABSTRACT

Uncertainties in the sub-nanometer range, the use of new materials, roughness, and the three-dimensional structures represent main challenges for the metrology of critical dimensions in nanostructures. In this paper, Monte Carlo modeling is used to investigate the correlation of the "true line edge roughness" of photoresist lines with the roughness rendered by Critical Dimension Scanning Electron Microscopy. Examples are presented, where realistic full-three dimensional photoresist structures in the nanometer range are generated by TCAD process simulation.

1. Introduction

Statistical fluctuations of the critical dimensions in the Front-End-of-Line represent a challenge for the yield and reliability of CMOS technologies in the sub-22 nm nodes. This implies the use of advanced characterization techniques with resolution capabilities in the sub-nanometer range. The line width roughness (LWR) of a structure such as a gate in an integrated circuit, is given by the variation of the nominal width, so called critical dimension (CD), along the main direction. The line edge roughness (LER) is defined analog to LWR by the variation of the one edge position of the line along the main direction of the structure. In the sub-nanometer range, LWR/LER are caused by different stochastic processes with a non-constant variance. The roughness has statistically significant effects on the performance of integrated circuits, therefore it needs to be properly characterized and controlled. As an example, the fluctuation of the gate width in a MOSFET causes a non-uniform distribution of the current density, which can turn into non-local temperature gradients across the channel. The roughness of the gate has also an impact on the drive and off-state leakage current [1]. Earlier studies [2] did show that high-frequency spectral components of the roughness have the most relevant effects on performance degradation, thus quantitative statistical and spectral analysis tools are needed.

Recently, it has been suggested [3] that there is no physical reason that would prevent the use of Critical Dimension Scanning Electron Microscopy (CD-SEM) for the metrology of three-dimensional lithography patterns in the sub-10 nm range. However, facing the challenges in terms of accuracy and uncertainty that are stated in the ITRS Metrology Roadmap implies an increased demand for optimized SEM equipment, better image acquisition strategies, as well as the implementation of shape-sensitive, model-based evaluation techniques. For these reasons, the intrinsic limitations of SEM have to be explored based on detailed physical modeling of the influence of proximity and self-charging effects, signal generation, as well as an accurate three-dimensional (3D) description in the nanometer-scale of the geometry of arbitrary and dense resist structures. At present, Monte Carlo (MC) modeling is still the technique of choice. Due to the limitations of existing MC simulators, the rendering of the LER by CD-SEM has been investigated for pseudo-3D structures only, where the statistical fluctuations of the critical dimensions only happen in the horizontal plane, but not in along the *z*-axis [8,9]. Thanks to the recent advances in MC simulation for SEM [5,6], it became feasible to simulate realistic 3D geometries generated by TCAD simulation, which can account for texture variations in all three-space directions.

2. Modeling methodology

2.1. Requirement to the simulation tool and state-of-the-art

A major culprit affecting MC simulation of realistic 3D samples is the long calculation time due to particle tracking, which is almost not sustainable for industrial applications. In addition, MC simulation of realistic samples by former tools required the use of different engines to edit the geometry by hand, to mesh the structure. Therefore, past simulation tools were often limited to

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samples modeled by sparse basic body geometries, in spite of the fact that real samples are complex and dense 3D volumes with heavily textured surfaces. Complex sample geometries are usually described by an unstructured mesh up to 2,000,000 tetrahedra. Thanks to a dedicated voxelization strategy [6], the calculation time required by MC tracking in densely meshed structures is typically just a factor of two larger than in geometries using basic bodies. This makes possible to calculate linescans and images of large-size 3D models at high resolution within minutes, or few hours and to compile dense model-based libraries as shown in Section 3.1.

2.2. Dedicated Monte Carlo simulation tool and TCAD

In present paper, the Monte Carlo Integrated Electron Beam Simulator (IES) developed at the ETH Zurich is used to simulate secondary electron images of photoresist structures in the nanometer scale. IES has been especially designed to accept complex sample geometries with Line Edge Roughness (LER) and to work within a commercial TCAD environment [4]. The physics considered in IES to simulate the electron-probe interactions has been presented in previous works [5,6] and recently extended to dielectrics. Special attention has been paid to the calculation time. Thanks to the use of efficient tracking algorithms and of advanced parallelization schemes, complex 3D samples can be simulated within minutes and some few hours. This enables the compilation of large libraries to be used for CD extraction. IES uses advanced parallelization schemes, such that it can be run on portable computers, workstations, computer clusters, as well as on number crunchers, like the petaflop supercomputer *Piz Daint* at the Swiss National Supercomputing Centre [7].

Besides the accurate modeling of the physical scattering mechanisms present application also needs a realistic description of the sample geometry to account for surface roughness, irregular shapes, and thin material layers. The traditional approach to the definition of complex geometries makes use of basic shapes. This represents a major limitation in 3D modeling. To solve this issue, in IES, a TCAD environment is used to define, visualize, and conveniently mesh complex geometries in the nanometer range, still keeping the computational effort under control. In the proposed application, the geometries used in IES are created by the TCAD lithography simulator SENTAURUS-Litho [4]. Thanks to these peculiarities of IES, for the first time, realistic SEM images of full-3D samples could be simulated to account for realistic textures of nanostructures.

2.3. Metrics for roughness

Roughness is a stochastic process with a finite variance. If N measurements of the local edge position (X_i) and of the linewidth (W_i) are acquired along the main axis of the line with nominally parallel edges at a constant sampling step size Δ, the deviation from the respective mean value (x_i and w_i, respectively) can be written as

$$x_i = X_i - \overline{X}; \quad w_i = W_i - \overline{W}$$

This leads to the definition of the Mean Square Roughness

$$\text{LER}: \hat{\sigma}_E^2 = \frac{1}{N-1}\sum_{i=1}^{N} x_i^2; \quad \text{LWR}: \hat{\sigma}_W^2 = \frac{1}{N-1}\sum_{i=1}^{N} w_i^2$$

$$\text{LER}: R_E = 3\sqrt{\hat{\sigma}_{E\_left}^2 + \hat{\sigma}_{E\_right}^2}; \quad \text{LWR}: R_W = 3\hat{\sigma}_w$$

where $\hat{\sigma}_{E\_left}$ and $\hat{\sigma}_{E\_right}$ represent the Mean Square Roughness of the positions along the left and right edge, respectively. The spectral information of the line with length L is obtained from the Power Spectrum of the LER and LWR, which delivers the amplitude of each frequency component of the roughness. As an example, the k complex coefficient of the discrete Fourier transform of the width residuals can be written as

$$a_k = \sum_{j=0}^{N-1} w_i \exp(-i2\pi jk/N) \qquad k = 0, \ldots N-1$$

Thus the power content at a given frequency f_k is expressed as

$$P(f_0) = \frac{\Delta}{N^2}|a_0|^2; \quad P(f_k) = \frac{\Delta}{N^2}[|a_k|^2 + |a_{N-k}|^2]; \quad P(f_{N/2}) = \frac{\Delta}{N^2}|a_{N/2}|^2$$

where Δ is the sampling step and $f_k = \frac{k}{N\Delta}$ with $f_{min} = \frac{1}{L}$ and $f_{max} = \frac{1}{2\Delta}$.

Since x_i and w_i are positive values, the Power Spectrum is symmetric to f_0. Based on the Parseval relation

$$\sum_{k=0}^{N-1} w_k^2 = \frac{1}{N\Delta}\sum_{k=0}^{N/2} P_k$$

LER and LWR can be also represented by the power component P_k at the frequency f_k, as follows

$$\text{LER}: R_E^2 = \frac{1}{(N-2)N\Delta}\sum_{k=0}^{N/2} P_k; \quad \text{LWR}: R_W^2 = \frac{1}{(N-1)N\Delta}\sum_{k=0}^{N/2} P_k$$

Thus, the Mean Square Roughness $\hat{\sigma}_E^2$ and $\hat{\sigma}_W^2$ can be easily obtained from the autocorrelation function c_E and c_W

$$\text{LER}: c_E(k) = \frac{1}{(N-2)\hat{\sigma}_E^2}\sum_{i=1}^{N} x_{i+k}x_i; \quad \text{LWR}: c_W(k) = \frac{1}{(N-1)\hat{\sigma}_W^2}\sum_{i=1}^{N} w_{i+k}w_i$$

2.4. MBLA and contour

In this paper, CD are extracted from simulated SEM images according either to the model-based library approach (MBLA), or by the contour technique.

The first step of the MBLA is the definition of model shapes. The most common model shapes are *Rectangular*, *Rounded top*, and *Tapered sidewall*. The following step of the procedure is the compilation of the model library for a given model shape, whose parameters (e.g. linewidth and pitch) are varied within predefined intervals. Each entry of the library consists of the linescan obtained from the simulation of the model shape for a given set of parameters. Once the library has been completely compiled, the extraction procedure consists of the comparison of the line under investigation with all library entries to find the "best match". This process is conveniently carried out by cross-correlation analysis. In fact, the cross correlation between two signals measures the similarity of the signals. For two arbitrary continuous signals $\varphi(x)$ and $\psi(x)$ the cross correlation can be written as

$$C(\tau) = \int_{-\infty}^{\infty} \varphi(x)\psi(x+\tau)dx$$

The best "correlation" is found at the value of the lag parameter τ, where $C(\tau)$ reaches its maximum. This procedure is much faster that alternative fitting techniques and delivers at the same time the best matching function as well as its shift from the origin.

The Contour technique applies usually to 2D SEM images, where the gray levels associated to each pixel are considered as the elevation of a pseudo-2D surface. The contour lines are then defined as the curve along which the surface assumes a constant value. Typical values are 20% and 80% of the peak intensity. Contour lines can be used either to estimate the distances in the SEM image (e.g. linewidth), or to quantify the roughness