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Effective medium approximation of ellipsometric response from random surface roughness simulated by finite-element method

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ABSTRACT

We used numerical simulations based on the finite-element method (FEM) to calculate both the amplitude and phase information of the scattered electric field from random rough surfaces, which can be directly compared to ellipsometric measurements and effective medium approximation (EMA) calculations. FEM can serve as an exploration tool for the relationship between the thickness of the surface roughness evaluated by Bruggeman EMA and the morphological parameters of the surface, such as the root mean square height, the lateral auto-correlation length, and the typical average slope. These investigations are of high interest in case of poly-crystalline and amorphous materials. The paper focuses on the simulations of rough Si surfaces. The ellipsometric calculations from FEM and EMA simulations match for wavelengths of illumination much shorter than the typical feature size of the surface. Furthermore, for these cases, the correlation between the EMA thickness and the root mean square height of the roughness for a given auto-correlation length is quadratic, rather than linear, which is in good agreement with experimental measurements and analytical calculations presented in recent reports.
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1. Introduction

Characterizing surface roughness with ellipsometry has become a routine practice since the birth of spectroscopic ellipsometry because of its fast, non-destructive, and in-line capabilities. The most widely used models describe the surface roughness with an effective medium approximation (EMA), i.e. the surface roughness is considered a homogeneous layer with an effective dielectric function mixed from the dielectric functions of the two media separating the rough interface. A good review about the relationship between surface morphology and EMA roughness can be found in Ref. [1]. Many experimental comparisons have been made between the EMA measured by ellipsometry and the morphology measured by atomic-force microscopy (AFM) for different Si samples: wet etched and thermally annealed Si [2], CVD deposited poly-Si [3,4], and poly-Si-on-oxide [5], as well as for in-situ growth of amorphous hydrogenated Si [6] and CVD deposited microcrystalline-Si on amorphous Si [7]. These works all concluded at a positive linear relationship between EMA roughness and AFM root mean square height, but all with different linear parameter values (slope and offset). One study even showed a negative correlation [8], stating that AFM measurements indicate an increase in root mean square height while ellipsometry suggests a smoothening of roughness. To better grasp the kaleidoscope of these different results, the present study simulates the ellipsometric response of a large number of random Si surfaces with well-defined root mean square heights and correlation lengths. The numerical simulations have been made by finite-element methods (FEM). FEM is a numerical technique to find approximate solutions of partial differential equations. Optical FEM is based directly on the linear Maxwell's equations in frequency domain. Computation of the electric (and the magnetic) field amplitudes are solved on a polygonal mesh, typically triangular, with piecewise-polynomial interpolation between the mesh points. Arbitrary geometrical objects can be defined with permittivity and permeability values assigned to each object (more specifically, assigned to the mesh points approximating the object). A summary of the vast areas of interest of the optical FEM can be found in Ref. [9]. The ellipsometric simulations of the random rough surfaces may be considered in our case as the “measured” samples and the effective medium roughness as the model to be fitted. This approach reveals many interesting effects concerning the relationship between the surface morphology and the thickness of the EMA roughness.

2. Model structures

Electromagnetic near fields resulting from plane wave illumination of silicon surfaces with roughness were simulated using the finite-

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element solver JCMSuite (version 2.16). Specular reflection amplitudes (and intensities) were obtained from far field results computed in post-process as a spatial (discrete) Fourier spectrum. Although the Maxwell equations are solved as stationary wave solutions in frequency domain, from the complex scattered electric fields, both the amplitude and phase information can be obtained. As the electric fields of the incident plane waves polarized parallel (P) and perpendicular (S) to the plane of incidence in the finite-element simulations are defined with unit amplitudes, the ellipsometric complex ρ is obtained as the ratio of the reflected complex amplitudes of the P and S polarizations. The ellipsometric angles are defined in the usual way as $\Psi = tan^{-1}(\rho)$ and $\Delta = arg(\rho)$, where $tan\ \Psi$ is the amplitude ratio and Δ is the phase difference, respectively, of the complex reflection coefficients of P and S polarized light [10,11]. The spectra were simulated in a wavelength range from 200 to 1000 nm, in steps of 10 nm, for the angles of incidence of 65° and 75°. The near-field amplitudes had to be computed individually for each wave vector of the illumination, because of the optical dispersion of the Si material [12].

For computational reduction, the simulation domain was 2-dimensional, with a translational symmetry in the direction perpendicular to the plane of incidence. This very useful simplification is based on the assumption that cross-polarizations due to the anisotropic nature of the simulated surface (as opposed to a real randomly rough 2D surface) are negligible, as the surface features are much smaller than the wavelength of light (λ). Furthermore, to eliminate scattering-like artifacts at the edge of the surface, periodic boundary conditions were used at these lateral sides of the computational domain. For the two remaining sides, transparent boundary condition was applied. The topographic points of the surface were generated with D. Bergström's Open Source MATLAB code [13] in such a way that the height distribution followed a Gaussian statistics. For visualization, a portion of the simulation mesh of a surface with a correlation length of 10 nm and a root mean square roughness of 2.5 nm is shown in Fig. 1a (left) with the height distribution histogram (right). An easy way to achieve such a height distribution is to convolute a predefined Gaussian filter on an uncorrelated (Gaussian) distribution of surface points generated by random numbers (i.e. white noise) [14]. The advantage of this approach is that the standard deviation of the uncorrelated distribution and of the Gaussian filter will be inherited and account for the root mean square height (R_{RMS}) and the correlation length (ξ) of the surface, respectively. Of course, due to the stochastic nature of the structure, small deviations will be present between the predefined standard deviations and the R_{RMS} values. To achieve adequate Gaussian statistics and diminish deviations from nominal values, the length of the surface to be simulated (L) was chosen such that $L/\xi \geq 500$. Additionally, L was at least 5 μm so that diffraction due to periodic boundary conditions would be negligible (parameter convergences as a function of L were studied). The simulated topographical parameters for ξ were 2.5, 5, 10, and 20 nm, while for the R_{RMS} were 0.5, 1, 1.5, 2.5, 3.5, 5, 7.5, 10, 15, and 20 nm. The combinations of all these parameter values are simulated, totaling in 40 points.

JCMSuite permits adaptive mesh refinement, i.e., after a pre-generated grid (following the curvature of the geometry), local grid refinements are applied as a function of the previously solved field amplitude gradients and a new refined mesh is calculated. These steps can be iterated to achieve adequate convergence and necessary precision. Faster convergences can be achieved when using higher FEM degrees. In our simulations, computational costs and ellipsometric angle convergences as a function of the refinement steps and the FEM

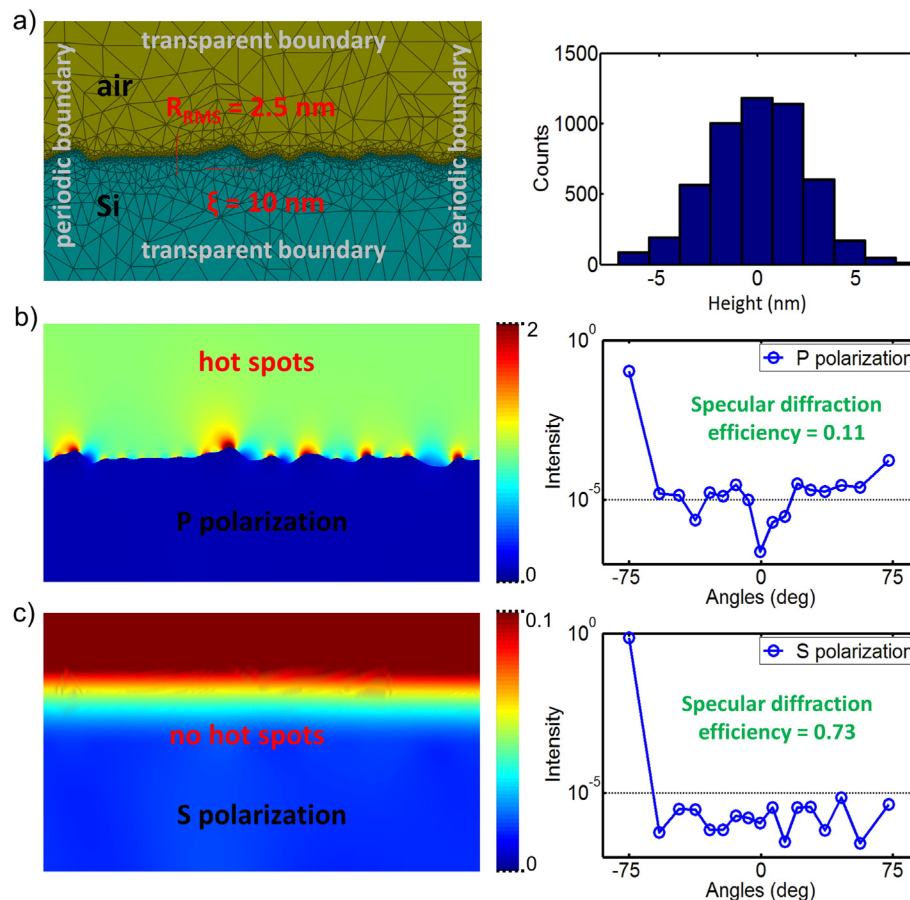

Fig. 1. Scattering simulation of one of the generated surface roughness for a plane wave incident at 75° at a wavelength of 600 nm. (a) Local grid structure after one refinement step (left) and the Gaussian distribution of surface heights (right). Near field intensity image and far field intensity angular distribution for (b) P polarization and for (c) S polarization (with −75° meaning the specular reflection).

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