Applied Surface Science 276 (2013) 447–453

Contents lists available at SciVerse ScienceDirect

Applied Surface Science

journal homepage: www.elsevier.com/locate/apsusc

Influence of non-Gaussian roughness on sputter depth profiles

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ARTICLE INFO

Article history:
Received 5 February 2013
Received in revised form 17 March 2013
Accepted 18 March 2013
Available online 27 March 2013

Keywords:
Surface and interface roughness
Height distribution function
MRI model
Sputter depth profiling
Non-Gaussian height distribution

ABSTRACT

Surface/interface roughness has a significant influence on the shape of the depth profile measured by any depth profiling technique. Such an influence is particularly significant for thin delta layers and at sharp interfaces of single- and multilayers. In the mixing-roughness-information (MRI) model for quantification of measured depth profiles, the influence of roughness is usually taken into account by a Gaussian height distribution function (HDF). If the roughness cannot be represented by a Gaussian HDF, a non-Gaussian HDF has to be implemented into the MRI model. Deviations of simulated depth profiles using the MRI model with Gaussian and with several well-defined non-Gaussian HDFs are evaluated quantitatively. The results indicate that a realistic non-Gaussian HDF has to be taken into account if high accuracy in quantification of sputter depth profiles is required. Of particular importance is the case of a roughness given by an asymmetrical HDF. Application of an asymmetrical triangle height distribution function in the MRI model yields an excellent fit for the measured AES depth profiling data of a polycrystalline Al film.

1. Introduction

The mixing-roughness-information (MRI) model is a versatile method for the quantification of sputter depth profiles measured by Auger electron spectroscopy (AES), X-ray photoelectron spectroscopy (XPS), secondary ion mass spectrometry (SIMS) and glow discharge optical emission spectroscopy (GDOES) depth profiling techniques [1]. Mathematically speaking, the sputter depth profile can be simulated by the convolution integral of the true compositional depth profile with a depth resolution function. This so-called depth resolution function is supposed to take into account *all* the distortional effects upon sputter depth profiling. In the MRI model, the depth resolution function is constructed by two exponential functions (i.e. g_w and g_λ) and one Gaussian function (g_σ) (see below), which represent the three major distortional effects existing in any sputter depth profiling experiment: atomic mixing (g_w) by ion bombardment, information depth (g_λ) of the analyzed species, and the surface and interface roughness (g_σ) of the specimen [2,3]. These three functions are characterized by the following three parameters: the atomic mixing length (w), the information depth (λ), and the roughness parameter (σ). Depending on the sputtering conditions, the values of these three MRI parameters can be taken as constant or as depth-dependent [4–7] for quantitative interpretation of depth profiling data.

In the MRI model, the roughness parameter is usually represented by a Gaussian function that is supported by surface height distribution measurements by atomic force microscope (AFM) [8,9] or by interfacial concentration distribution measurements by grazing incidence X-ray reflectivity (GIXR) [10,11]. However, in some cases, the surface height distribution may be presented by a non-Gaussian function, such as due to sputtering induced roughness [12] and ripple formation/patterned surface [13–15], crystallite orientation dependent sputtering yield [16], second phase particles and chemical surface etching [17]. When the areal distribution of surface parts with different heights within the analyzed area is not represented by a Gaussian distribution (or that of the corresponding concentration distribution at an interface), the question arises about the magnitude of the influence of the latter on quantitative profile evaluation. To answer this question, we have implemented in the MRI model three non-Gaussian height distribution functions (HDFs) given by an isosceles triangle, an isosceles trapezoid and a right-angled triangle, and evaluated quantitatively the respective deviations between the sputter depth profiles calculated with the latter and that calculated with the usual Gaussian HDF.

2. Gaussian and non-Gaussian height distribution functions

The surface topography of specimens is generally characterized by AFM or surface profilometry via the so-called surface roughness

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http://dx.doi.org/10.1016/j.apsusc.2013.03.114

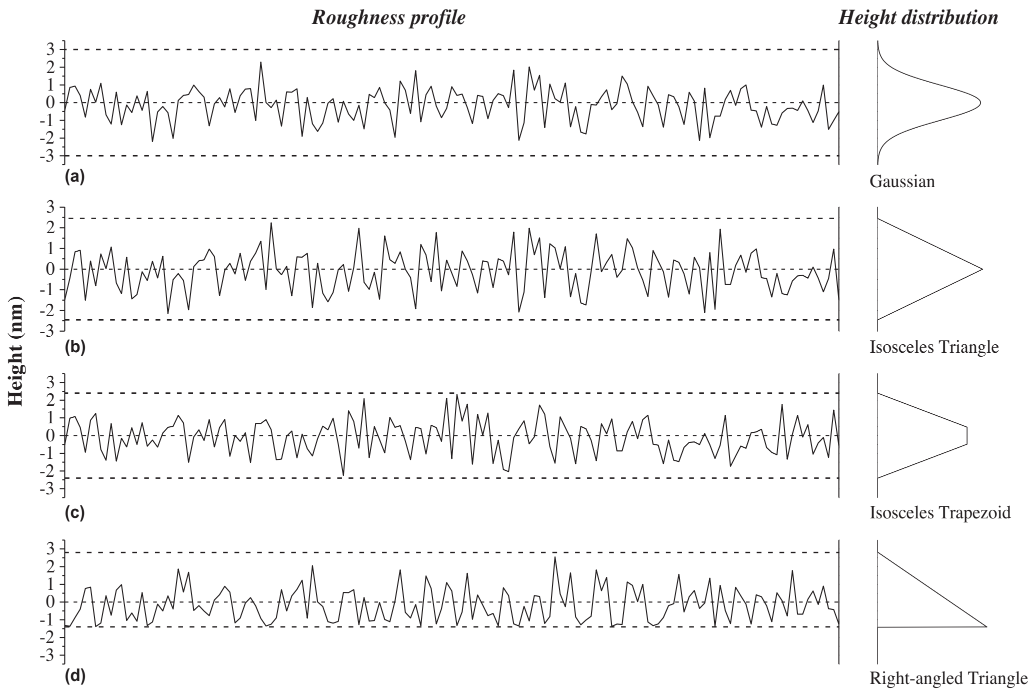

Fig. 1. The roughness profiles (the left parts) and the corresponding height distributions (the right parts): (a) Gaussian, (b) isosceles triangle, (c) isosceles trapezoid, and (d) right-angled triangle. The mean line is indicated as the dashed line located at the height of zero. The two dashed lines above and below the mean line represent the maximum and the minimum lines, respectively.

profile that is a measure of the surface height perpendicular to the average surface height (mean line) as the simulated one shown in the left part of Fig. 1. The mean line can be determined either by $\bar{z} = \frac{\sum_{i}^{n} z_i}{n}$ from the measured roughness profile or by $\bar{z} = \int_{-\infty}^{+\infty} zp(z)dz$ from the given HDF of $p(z)$. In general, the mean line is set at the location of $z = 0$ as indicated in the left part of Fig. 1.

The surface height distribution (histogram of surface height) can be extracted from the measured roughness profile and is shown in the right part of Fig. 1. This surface height distribution function (HDF) can be regarded as a representative of the specimen roughness in depth profiling if the sputtering rate in the analyzed area is constant.

In the MRI model, the depth resolution function representing the roughness induced broadening effect is described by a Gaussian function as [1–3]:

$$g_\sigma = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[\frac{-(z-z_0)^2}{2\sigma^2}\right] \quad (1)$$

where z_0 is the position of sputtered depth, the standard deviation σ denotes the surface or interface roughness parameter, and z is an independent parameter having the length dimension of the convolution operation.

The normalized isosceles triangle function $g_{\sigma\text{-}ITRI}$ with the same characteristic parameter σ and the same height as that of function g_σ is given by:

$$g_{\sigma-ITRI} = \begin{cases} \frac{1}{2\pi\sigma^2}(z-z_0) + \frac{1}{\sqrt{2\pi}\sigma} & -\sqrt{2\pi}\sigma < z - z_0 < 0 \\ -\frac{1}{2\pi\sigma^2}(z-z_0) + \frac{1}{\sqrt{2\pi}\sigma} & 0 \le z - z_0 < \sqrt{2\pi}\sigma \\ 0 & \text{Otherwise} \end{cases} \quad (2)$$

where σ denotes a characteristic roughness extension parameter which is defined by half of the baseline of the isosceles triangle through $L/2 = \sqrt{2\pi}\sigma$ (see Fig. 2).

For the normalized isosceles trapezoid function, the ratio of the top horizontal line to the baseline is assumed as $L_{top}/L = 0.2$ and the height H is the same as that of the Gaussian function ($H = 1/(\sqrt{2\pi}\sigma)$). Such an isosceles trapezoid function $g_{\sigma\text{-}ITRA}$ is given by:

$$g_{\sigma-ITRA} = \begin{cases} H & -0.1L \le z - z_0 \le 0.1L \\ 1.5H^2(z-z_0) + 1.25H & -0.5L < z - z_0 < -0.1L \\ -1.5H^2(z-z_0) + 1.25H & 0.1L < z - z_0 < 0.5L \\ 0 & \text{Otherwise} \end{cases} \quad (3)$$

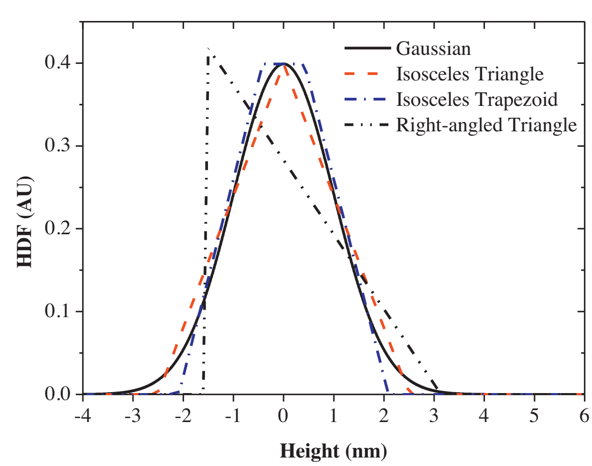

Fig. 2. Different height distributions: Gaussian (solid line), isosceles triangle (dashed line), isosceles trapezoid (dashed dotted line) and right-angled triangle (dashed double-dotted line) calculated from Eqs. (1)–(4), respectively, for $\sigma = 1$ nm and $z_0 = 0$.