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Determination of the X-ray mirror component angle dependence and effective surface roughness on the basis of AFM measurements

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Abstract: We report the results of comparative investigations of the glass substrates surface roughness by atomic-force microscopy (AFM) and X-ray reflectivity (XR) methods. Based on the AFM data, the parameters of the effective roughness that determines reflectivity of X-ray radiation have been calculated. It is shown that the effective rms roughness values and angular dependencies of the reflection coefficient in the X-ray wavelengths range, calculated from the AFM profiles of substrates surface, are in good agreement with the XR measurement data.

Introduction

Atomic-force microscopy and X-ray reflectometry are widely used in study of surface roughness on a nanometer scale. It has been established to date that both these methods as applied to supersmooth surfaces ensure good agreement of the results in measurements of an rms deviation of the roughness heights [1,2]. For surfaces with a well-developed relief, that feature a largely non-Gaussian height distribution, a sharp discrepancy between XR and AFM measurements data was observed [3,4]. In [4] it was suggested that the reflectivity of X-ray radiation from a surface is mainly determined by the Gaussian relief component. A method was proposed to calculate the parameters of X-rays reflectivity from a rough surface on the basis of AFM profile measurements, which allowed to determine the effective surface roughness in the X-ray range of wavelengths. In this work we present the results of the XR and AFM assisted comparative studies on the surface roughness of glass substrates.

Experiment

Three glass substrates varying in a type of surface roughness were selected as test samples. Surface relief was investigated on a “Solver” AFM (designed and manufactured by the NT-MDT Company, Zelenograd, Russia). The maximum scan area was 40 x 40 μm; a frame was a data array of 512 x 512 elements. In study of the substrates roughness we took a series of equal-size frames from different parts of the surface. For each frame we calculated the parameters of rms deviation of the relief heights, σ_{AFM}. Also, measurements were made on an X-ray diffractometer in the hard X-rays range Cu-K_α (λ = 0.154 nm) for sliding angles close to 0^0. The effect of the X-rays scattering on surface roughness was taken into account in the expression for the reflectivity through the Debye-Waller exponential factor [5]:

$$R = R_o\, exp(-\sigma_{XR}{}^2\, q^2),$$

where R_o is the ideal surface reflectivity calculated by the Fresnel equations, $q = 4\pi\lambda^{-1}\sin\alpha$ is the scattering vector component normal to surface, α is the sliding angle, σ_{XR} the parameter describing the surface roughness in the X-ray range of wavelengths.

Results and Discussion

Our investigations have shown the parameter σ_{AFM} derived from the AFM measurements to be largely dependent on the scan area size. Fig.1 (a,b) shows the rms deviation parameter and the AFM measured roughness versus a frame size. The surfaces with largely non-Gaussian height distribution reveal a considerable difference in their values of σ_{AFM} and parameter σ_{XR} obtained by XR measurements.

Fig. 1. Scale dependence of the parameters characterizing surface roughness, on AFM frame size L for the Gauss (a) and non-Gauss (b) substrate surfaces. Curve (1) is for parameter σ_{AFM}, (2) is the dependence of parameter σ_{eff} on a frame size. Dashed line (3) denotes the value of σ_{XR} obtained from the X-ray measurements.

As shown in [4], the X-rays scattering is mainly determined by the Gauss component of surface relief $z = f(x,y)$ and is described by the scattering factor in the following form:

$$\psi(q) = \left| \frac{1}{S} \int_S e^{iqf(x,y)} dxdy \right|^2$$

where S is the area of a frame. This factor has an angular dependence, which is similar to the Gauss curve with some effective parameter for roughness.

Rigorously speaking, the definition for the effective rms roughness is somewhat conventional in the case of X-ray reflectivity on strongly non-Gauss surfaces. Here the quantity

$$\sigma_{eff} = \sqrt{-\frac{1}{q^2} \ln \psi(q)}$$

is the incidence angle function and, hence, we only may have some average value of the rms roughness of surface in the some interval of angles. Fig. 2 is the dependence of σ_{eff} on parameter q for one AFM image of surface. As follows from the calculations, the parameter σ_{eff} averaged over the angle interval exceeding the critical one also has a scale dependence on a frame size (Fig.1), but the estimates for the average value of σ_{eff} for non-Gauss surface are closer to the experimental value of σ_{XR}. As for the Gauss type surface, the averaged σ_{eff} value practically coincides with σ_{AFM} and is getting closer to σ_{XR} with the scan area increasing. Thus, as is quite well seen from Fig. 1, a large scan area should be used for the effective surface roughness σ_{eff} determination.

Using the AFM data and Fresnel equations, we derived angular dependencies of the X-rays reflection coefficients in the region of sliding angles close to 0^o for all substrates. Fig. 3 shows such dependencies calculated from the AFM surface images of one substrate. It is nicely seen that the angular dependence derived directly from the AFM image of surface relief is in good agreement with the experimental curve obtained by XR measurements.

Fig. 2. Angular dependence of the effective roughness calculated directly from the AFM image of surface relief. The part of the *q* range from 0.05 to 0.1, corresponding to angles above the critical value, was taken for average σ_{eff} calculation.

Fig. 3. Angular dependence of X-rays reflectivity on a glass substrate surface. Curve (1) is the experimental dependence obtained in XR measurements; curve (2) is derived using the Debye-Waller dependence with parameter σ_{AFM} taken from AFM measurements. Curve (3) is calculated based on the scattering factor $\psi(q)$ calculated directly from the same the 40 × 40 μm AFM image of surface.

Conclusion

The methods of X-ray reflectivity and atomic-force microscopy were applied to investigate surface roughness of glass plates with different types of roughness. A sharp discrepancy was found between the estimates of the rms roughness of substrates, obtained from angular dependencies of the X-ray reflection coefficient and from statistical calculations based on AFM profiles of surface. This discrepancy is explained by the fact that the surfaces under study have essentially a non-Gauss type of roughness. The AFM measurement data for a series of substrates were used to calculate scale dependencies of the effective rms roughness affecting reflectivity in the X-ray region of wavelengths. It is shown that the average values of the effective rms roughness and the angular dependence of reflectivity in the X-ray region, calculated directly from the AFM surface profiles of glass substrates, are in good agreement with the results of X-ray measurements.

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