Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Structural reliability evaluation for low-*k* nanoporous dielectric interlayers integrated into microelectronic device

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GIXS Data Analysis

The intensity of GIXS (I_{GIXS}) from structures in a thin film can be expressed by a scattering formula:[1-5]

$$I_{\mathrm{GIXS}}(\alpha_{\mathrm{f}},2\theta_{\mathrm{f}}) \cong \frac{1}{16\pi^2}\cdot\frac{1-e^{-2\,\mathrm{Im}(q_z)t}}{2\,\mathrm{Im}(q_z)}\cdot\begin{bmatrix} |T_{\mathrm{i}}T_{\mathrm{f}}|^2 I_1(q_{\|},\mathrm{Re}(q_{1,z})) + \\ |T_{\mathrm{i}}R_{\mathrm{f}}|^2 I_1(q_{\|},\mathrm{Re}(q_{2,z})) + \\ |T_{\mathrm{f}}R_{\mathrm{i}}|^2 I_1(q_{\|},\mathrm{Re}(q_{3,z})) + \\ |R_{\mathrm{i}}R_{\mathrm{f}}|^2 I_1(q_{\|},\mathrm{Re}(q_{4,z})) \end{bmatrix} \quad (1)$$

where α_{f} and $2\theta_{\mathrm{f}}$ are the out-of-plane and in-plane exit angle of the out-going X-ray beam respectively, $\mathrm{Im}(q_z) = |\mathrm{Im}(k_{z,\mathrm{f}})| + |\mathrm{Im}(k_{z,\mathrm{i}})|$, Re($x$) is the real part of x, t is the film thickness, R_{i} and T_{i}

are the reflected and transmitted amplitudes of the incoming X-ray beam respectively, and R_f and T_f are the reflected and transmitted amplitudes of the outgoing X-ray beam respectively. In addition, $q_{||} = \sqrt{q_x^2 + q_y^2}$, $q_{1,z} = k_{z,f} - k_{z,i}$, $q_{2,z} = - k_{z,f} - k_{z,i}$, $q_{3,z} = k_{z,f} + k_{z,i}$, and $q_{4,z} = - k_{z,f} + k_{z,i}$; here, $k_{z,i}$ is the z-component of the wave vector of the incoming X-ray beam, which is given by $k_{z,i} = k_o \sqrt{n_R^2 - \cos^2 \alpha_i}$, and $k_{z,f}$ is the z-component of the wave vector of the outgoing X-ray beam, which is given by $k_{z,f} = k_o \sqrt{n_R^2 - \cos^2 \alpha_f}$, where $k_o = 2\pi / \lambda$, λ is the wavelength of the X-ray beam, n_R is the refractive index of the film given by $n_R = 1 - \delta + i\zeta$ with dispersion δ and absorption ζ, and α_i is the out-of-plane grazing incident angle of the incoming X-ray beam. q_x, q_y, and q_z are the components of the scattering vector **q**. I_1 is the scattering intensity of the structure in the film, which can be calculated kinematically.

In eq 1, I_1 is the scattered intensity from morphological structures (i.e., pores) in the low-*k* layer. To analyze the measured scattering patterns by using the above GIXS formula, we examined all possible scattering models, for examples, sphere, ellipsoid, cylinder, and so on. Then we found that a sphere model is the most suitable for the pores imprinted in the low-*k* layers, which can be expressed in the following equation:[1-7]

$$I_1 = c\int_0^\infty n(r)\upsilon^2(r)\,|\,F(qr)\,|^2\; S(qr)dr \tag{2}$$

where c is a constant, $n(r)$ is the radius r distribution of pores, $\upsilon(r)$ is the volume of each pore, $F(qr)$ is the form factor of pore (i.e., spherical form factor), and $S(qr)$ is the structure factor of pores where q is the magnitude of scattering vector **q**. For a hard sphere (i.e., spherical pore with a radius r), the form factor $F(qr)$ in eq 2 can be expressed in the following equation:[6,7]

$$F(qr) = 4\pi r^2 \cdot \frac{\sin(qr) - qr\cos(qr)}{q^3 r^3} \quad . \tag{3}$$

For hard spheres (i.e., pores) monodispered locally, their structure factor $S(qr)$ can be expressed by the following equation:[8]

$$S(qr) = \frac{1}{1 + 24\phi_p \cdot \frac{G(A)}{A}} \tag{4}$$

where $A = 2qr$ and ϕ_p is the volume fraction of pores. $G(A)$ is given as

$$\begin{aligned} G(A) &= \frac{\alpha}{A^2}(\sin A - A\cos A) + \frac{\beta}{A^3}\left[2A\sin A + (2 - A^2)\cos A - 2\right] \\ &+ \frac{\gamma}{A^5}\left\{-A^4\cos A + 4\left[(3A^2 - 6)\cos A + (A^3 - 6A)\sin A + 6\right]\right\} \end{aligned} \tag{5}$$

where

$$\alpha = \frac{(1 + 2\phi_p)^2}{(1 - \phi_p)^4} \tag{6a}$$

$$\beta = -6\phi_p \cdot \frac{(1 + \phi_p / 2)^2}{(1 - \phi_p)^4} \tag{6b}$$

$$\gamma = \frac{\phi_p (1 + 2\phi_p)^2}{2(1 - \phi_p)^4} \quad . \tag{6c}$$

In the data analysis, we found that the pores have a radius distribution following a lognormal function:[1-5]

$$n(r) = \frac{1}{\sqrt{2\pi}\, r_o \sigma e^{\sigma^2/2}} e^{\frac{-\ln(r/r_o)^2}{2\sigma^2}} \tag{7}$$

where r_0 and σ are the radius corresponding to the peak maximum and the width of the radius distribution of the pores respectively.

All GIXS data were successfully analyzed using the GIXS formula (eq 1) together with eq 2-7. The data analysis results are shown in Fig. 1 and Table 2.

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