Electronic Supplementary Material (ESI) for Soft Matter.

SUPPORTING INFORMATION

Prediction of time-dependent swelling of flexible polymer substrates using hygro-mechanical finite element simulations

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1. Constitutive equation for moisture absorption analysis model

In order to predict time-dependent hygroscopic deformation, it is critical to precisely evaluate the moisture distribution inside polymer substrates. The primary mechanism that moisture penetrates into polymeric materials is diffusion phenomenon described by Fick's law, which is expressed as follows:

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right), \tag{1}$$

where C, t, and D are the moisture concentration, time, and moisture diffusivity, respectively.

This equation can also be represented by the percentage moisture content, M, applied in this study as main parameter for moisture, and rewritten as follows:[1-3]

$$\frac{\partial M}{\partial t} = D\left(\frac{\partial^2 M}{\partial x^2} + \frac{\partial^2 M}{\partial y^2} + \frac{\partial^2 M}{\partial z^2}\right). \tag{2}$$

By solving this partial differential equation, the moisture content distribution can be quantitatively obtained depending on the diffusion time and position. However, in the cases of the problems including interfaces between different materials, they have discontinuities at the interfaces, because the saturated moisture contents are different between the materials.[1, 4-8] In order to solve such problems, the FEM code (ABAQUS ver. 6.12-1) that is employed in this study uses normalized approach,[9] which is a method to resolve interfacial discontinuity in multi-material problems by normalizing the moisture quantity parameter.[1,4-9] Therefore, the normalized variable is continuous between the different materials. As a normalized parameter, wetness is applied in this study, and this parameter is defined as follows:[3, 4, 6, 10, 11]

$$w = \frac{M}{M_\infty}, \tag{3}$$

where w and M_∞ denote wetness and saturated moisture content, respectively. Because wetness is normalized variable with saturated moisture content, it has a value between $0 \leq w \leq 1$, where w is 0 for fully dry condition and 1 for fully saturated condition. Using this normalized parameter, Eq. (2) can be represented as follows:

$$\frac{\partial (wM_\infty)}{\partial t} = D\nabla^2 (wM_\infty) \tag{4}$$

$$w\frac{\partial M_\infty}{\partial t} + M_\infty \frac{\partial w}{\partial t} = D(w\nabla^2 M_\infty + 2\nabla w \nabla M_\infty + M_\infty \nabla^2 w). \tag{5}$$

Saturated moisture content is linearly proportional to the relative humidity. This linear relationship is originated from Henry's law and is expressed as follows:[3, 8]

$$M_\infty \cong K(RH), \tag{6}$$

where K and RH are constant and relative humidity, respectively. Because this study was performed at fixed relative humidity of 95% RH, saturated moisture content is constant. Moreover, it can be assumed that this hygroscopic parameter is not dependent on the position inside the polymer substrates. Therefore, rearranging Eq. (5) with the constant M_∞ over time and position gives

$$\frac{\partial w}{\partial t} = D\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2}\right). \tag{7}$$

Because it is assumed that in initial stage the polymer substrates are fully dried and moisture can only diffuse through the side and bottom surfaces of substrates, fully dried initial condition inside polymer substrates and fully saturated boundary conditions for the side and bottom surfaces under 95% RH were applied as shown in Fig. S1a and b, and the mathematical expressions are as follows:

$$\text{Initial condition}: w(-l \le x \le l, 0 \le y \le h_{Sub.}, -a \le z \le a) = 0, \quad t=0 \tag{8}$$

$$\text{Boundary conditions}: w(x,0,z) = w(\pm l, y \le h_{Sub.}, z) = w(x, y \le h_{Sub.}, \pm a) = 1, \quad t>0. \tag{9}$$

Applying these initial and boundary conditions, the time-dependent moisture distribution was evaluated by the FEM code mentioned above, and hence the results were imported into each node of the mechanical model to quantitatively analyze the hygroscopic deformation behavior.

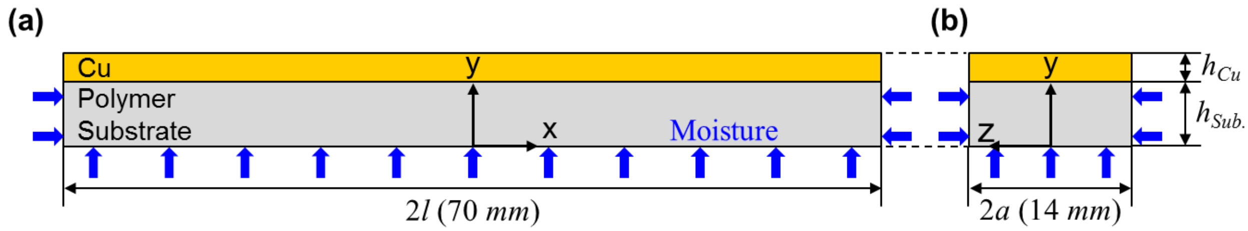

Figure S1. Schematics of boundary conditions for moisture absorption analysis: (a) front and (b) side views of the bilayer model.

2. Constitutive equation for mechanical analysis model

Hygroscopic strain is linearly proportional to the moisture content, and this relationship is represented as follows:[3, 12-14]

$$\varepsilon_{ij}{}^{h} = \beta M \delta_{ij}, \tag{10}$$

where $\varepsilon_{ij}{}^{h}$, β,M, and δ_{ij} are hygroscopic strain tensor, coefficient of moisture expansion, moisture content, and kronecker delta, respectively. The total strain, ε_{ij}, including mechanical strain, $\varepsilon_{ij}{}^{M}$, can be written as follows:

$$\varepsilon_{ij} = \varepsilon_{ij}{}^{M} + \varepsilon_{ij}{}^{h}. \tag{11}$$

Then, the constitutive relationship between stress and strain for isotropic linear elastic material can be expressed as follows:[15]

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}{}^{M} = C_{ijkl}(\varepsilon_{kl} - \varepsilon_{kl}{}^{h}) = C_{ijkl}(\varepsilon_{kl} - \beta M \delta_{kl}), \tag{12}$$

where $$C_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}),$$

$$\lambda = \frac{\nu E}{(1+\upsilon)(1-2\upsilon)}, \qquad \mu = \frac{E}{2(1+\nu)},$$

σ_{ij}, v, and E denote the fourth-order elastic tensor, lamé constants (λ and μ), stress tensor, Poisson's ratio, and elastic modulus, respectively. Eq. (12) can be rearranged as follows:

$$\sigma_{ij} = \lambda \varepsilon_{kk} \delta_{ij} + 2\mu \varepsilon_{ij} - \frac{E}{(1-2\upsilon)} \beta M \delta_{ij}. \tag{13}$$

The elastic modulus, Poisson's ratio, coefficient of moisture expansion, and moisture content are obtained by three-point bending test, substrates manufacturer's data sheet, moisture absorption test, and finite element simulation, respectively.

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