

Supporting information

Improvement of wood material properties via in-situ polymerization of styrene into tosylated cell walls

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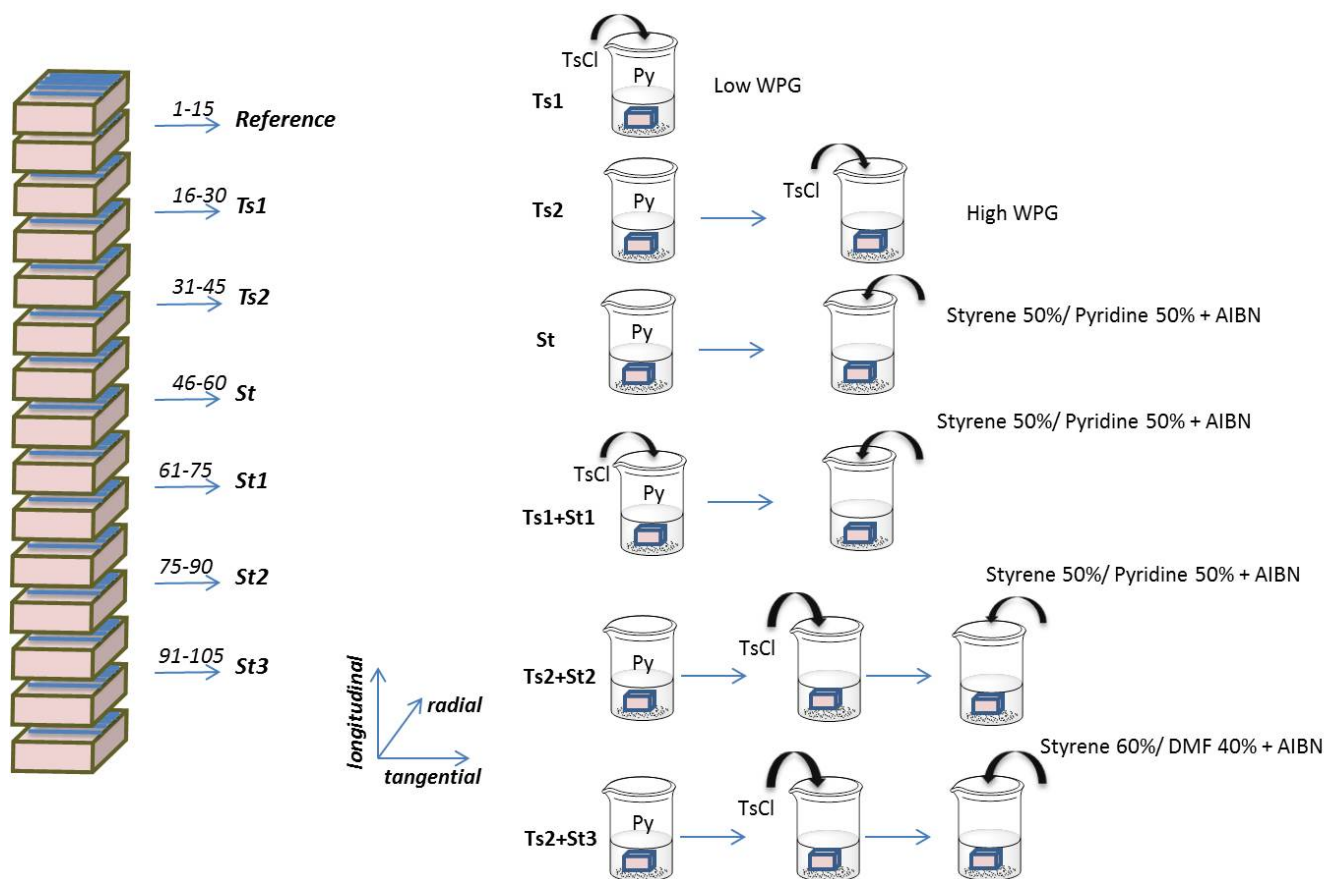


Figure S1. Left: wood sampling: fifteen (1x1x0.5 cm³) wood cubes for each set cut from spruce, in the longitudinal direction. Right: schematic representation of experimental flow. Ts1 (tosylation – low WPG), Ts2 (tosylation – high WPG), St (Styrene polymerization without tosylation pre-treatment), St1 (low WPG tosylation + styrene polymerization), St2 (high WPG tosylation + styrene polymerization), St3 (high WPG tosylation + styrene polymerization).

$S(\%) = \frac{(V_i - V_{ii})}{V_{ii}} \times 100$ <p>where S(%): volumetric swelling; V_i: wood volume after wetting with liquid water; V_{ii}: wood volume of oven-dried samples before wetting</p>	$ASE(\%) = \frac{S_{um} - S_m}{S_{um}} \times 100$ <p>where ASE(%): antishrinking/antiswelling efficiency resultin from the modification; S_m: modified volumetric swelling coefficient; S_{um}: unmodified volumetric swelling coefficient.</p>	$WU(\%) = \frac{(w_{ii} - w_i)}{w_i} \times 100$ <p>where WU(%): percentage of water uptake of the samples; w_i: initial weight of the sample; w_{ii}: wet weight of the sample after water-soaking</p>
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Figure S2. Equations for Swelling (S), Anti-swelling efficiency (ASE), and Water Uptake (WU)

$$EMC(\%) = \frac{(m - m_{od})}{m_{od}} \times 100$$

where EMC: is the moisture content;
m is the mass of the wood (with moisture) and
m_{od} is the oven-dry mass of the wood (i.e. no moisture)

Figure S3. Equation for Equilibrium Moisture Content (EMC).

Raman imaging and spectroscopy - Advanced Fitting tool:

The tool for advanced fitting (WitecPlus software) allows spectra to be fitted with Gaussian curve function. First dataset was background subtracted, and used to fit polystyrene curve at 1005 cm⁻¹ to the data set by keeping the width of the curve constant.

$$(a) \quad y = y_0 + \sum_{i=0}^{n-1} Amp_i e^{-0.5 \left(\frac{x - x_i}{s_i} \right)^2}$$

$$w_i = s_i \sqrt{8 \ln(2)}$$

$$A_i = Amp_i s_i \sqrt{2\pi}$$

n = Number of Gauss Functions

y_0 = Offset

x_i = Center

s_i = Width (Standard Deviation)

Amp_i = Amplitude

w_i = Width (FWHM)

A_i = Area

(b)

Parameters					
Name	Auto	Start Value	<< >>	Value	Vary
y0	<input type="checkbox"/>	10		10	<input type="checkbox"/>
x0	<input type="checkbox"/>	1005.0214		1005.0214	<input type="checkbox"/>
s	<input type="checkbox"/>	4.5		4.5	<input type="checkbox"/>
Amp	<input checked="" type="checkbox"/>	31.222355		31.222355	<input checked="" type="checkbox"/>

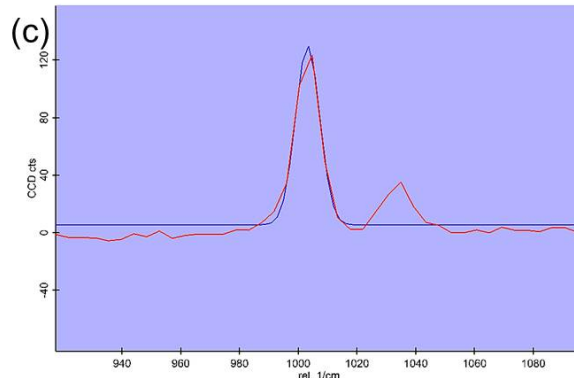


Figure S4: (a) Gaussian function and nomenclature of parameters used in the function. (b) parameter values to obtain related polystyrene image. (c) Gaussian fit of polystyrene curve at 1005 cm⁻¹ in the data set.

WPG% / Area Fraction Analysis:

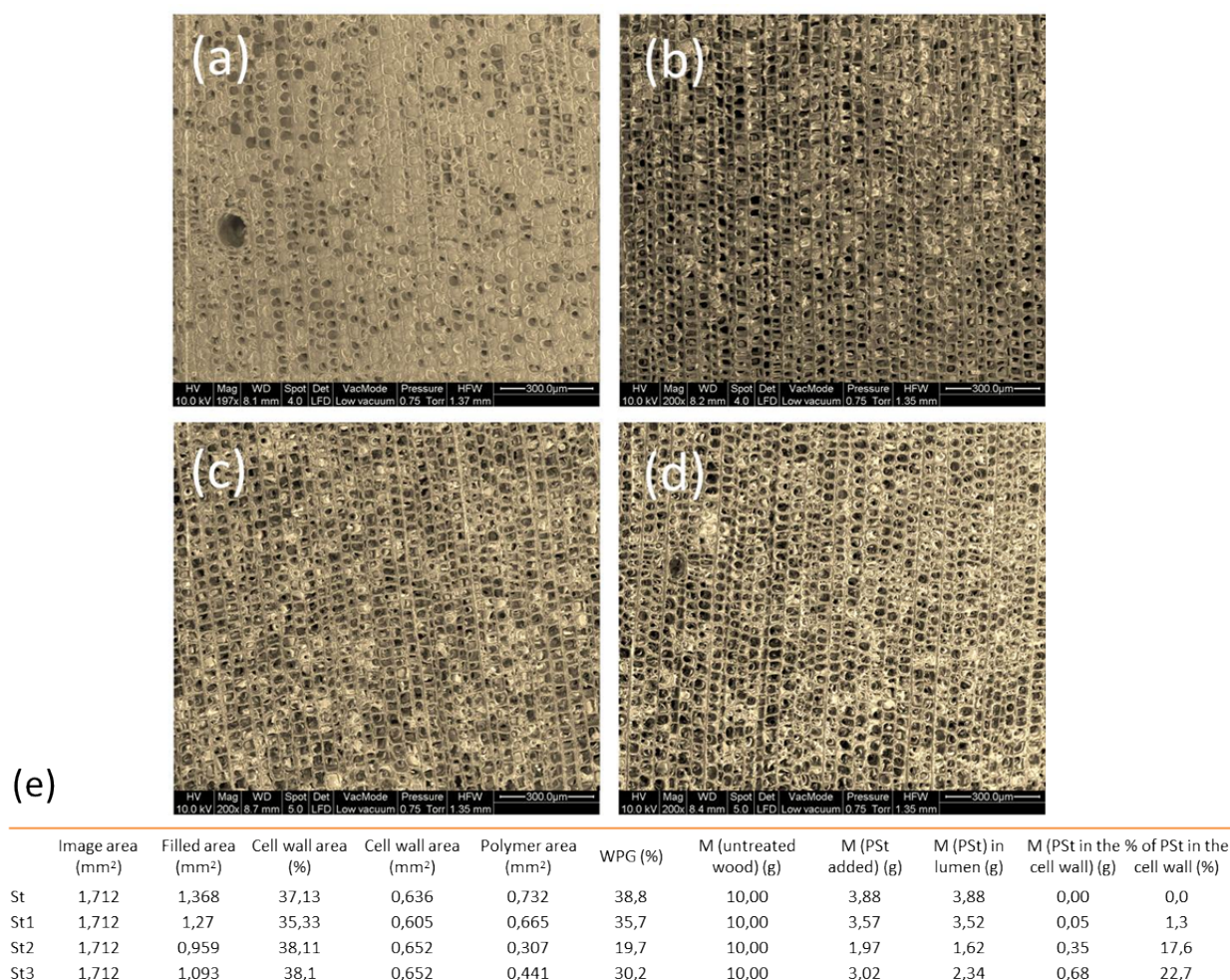


Figure S5: SEM images of (a) St, (b) St1, (c) St2, and (d) St3 samples used for semi-quantitative polymer WPG% determination in the cell walls. (e) WPG% and area values to calculate polymer content in cell walls.

From the SEM pictures, we can determine the area occupied by the cell wall material (Cell wall area), and the area occupied by the polymer in the lumen (Polymer area).

$$(Polymer\ area) = (Filled\ area) - (Cell\ wall\ area)$$

From the total weight percent gain determined after full modification, we know exactly how much polymer (in grams) was added to the wood. Assuming that for experiment St (no pretreatment), the polymer added is only located in the lumen part (which is consistent with literature), we can calculate the amount of polymer located in the lumen of other experiments (M (PSt) in lumen) as a function of the area occupied by the polymer on the SEM picture.

$$(M\ (PSt)\ in\ lumen) = (Polymer\ area\ of\ St1) / (Polymer\ area\ of\ St) \times (M\ (PSt)\ in\ lumen\ for\ St)$$

Once we have the weight of polymer in the lumen, we can get to the weight of polymer in the cell wall since we know the total amount of polymer:

$$M(PSt\ in\ the\ cell\ wall) = M\ (PSt\ added) - M(PSt\ in\ the\ lumen)$$

$$\% \ of\ Pst\ in\ the\ cell\ wall = M\ (Pst\ in\ the\ cell\ wall) / M\ (Pst\ added) \times 100$$