Chemical, Physical and Mechanical Characterization of Isocyanate-crosslinked Amine-modified Silica Aerogels

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Supporting Information

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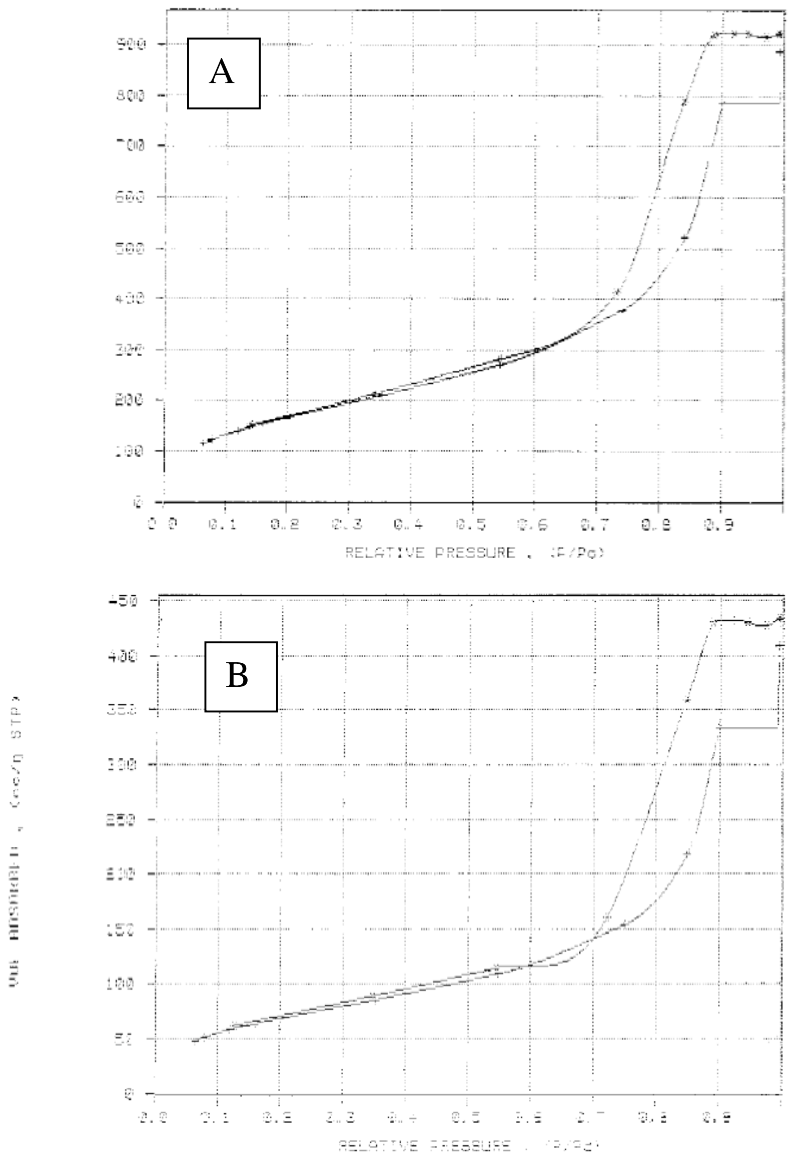

Figure S.1 Nitrogen adsorption isotherms for native amine-modified silica aerogels ($\rho \sim 0.19$ g cm^{-3}) (A), and isocyanate-crosslinked, amine-modified silica aerogels ($\rho \sim 0.48$ g cm^{-3}) (B).

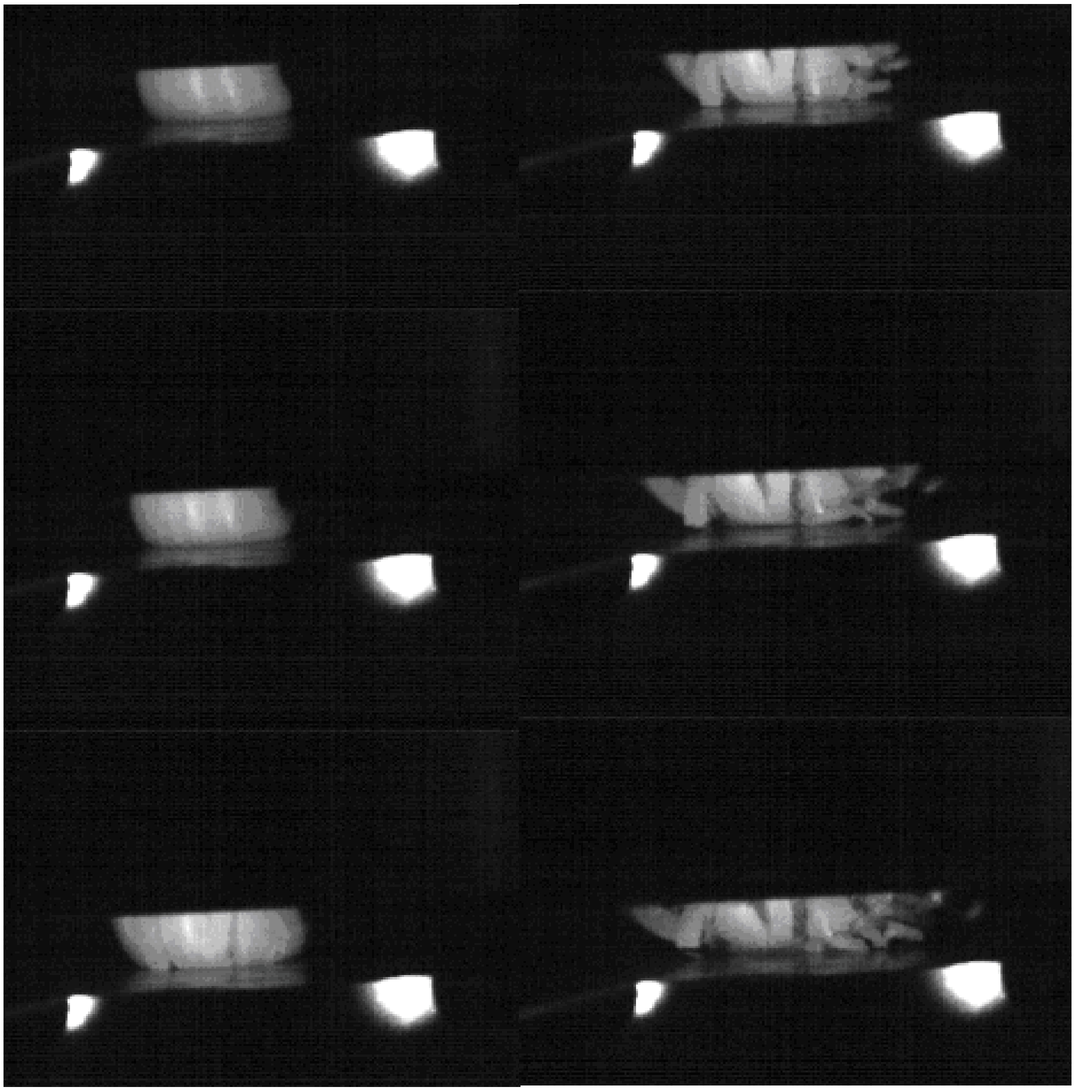

Figure S.2 Images using a high-speed camera to capture the crack initiation and failure under compression of an isocyanate-crosslinked, amine-modified silica aerogel sample ($\rho \sim 0.48$ g cm^{-3}). The crack initiation zones first appear as lighter areas running vertically through the sample.

Table S.1: Comparison of specific compressive strength of isocyanate crosslinked amine-modified silica aerogels with various materials[1,2]

Material	*Density (g/cm^{-3})*	*Compressive (Yield) Strength/ Compressive Stress at Ultimate Failure (MPa)*	*Specific Compressive Yield Strength / Compressive Stress at Ultimate Failure (Nm/Kg)*
E-glass epoxy*	1.94	550/550	283000/283000
Kevlar-49 epoxy*	1.30	280/280	215000/215000
T 300 epoxy*	1.47	830/830	564000/564000
VSB-32 epoxy*	1.63	690/690	423000/423000
GY-70 epoxy*	1.61	620/620	385000/385000
2024-T3 Al	2.87	310/345	108000/120000
7075-T6	2.80	542/593	194000/212000
4130 steel	7.84	436/1100	55600/140000
Crosslinked aerogel	**0.48**	**4.26/186**	**8900/389000**

* Fiber volume fraction V_f=0.6

1. *ASM Engineering Materials Handbook, Composites, Volume 1,* May 1988, Table 2, p 178.

2. Shigley, J. E.; Mischke, C. R. M. *Mechanical Engineering Design, 6th Edition*, 2001, p 1206.

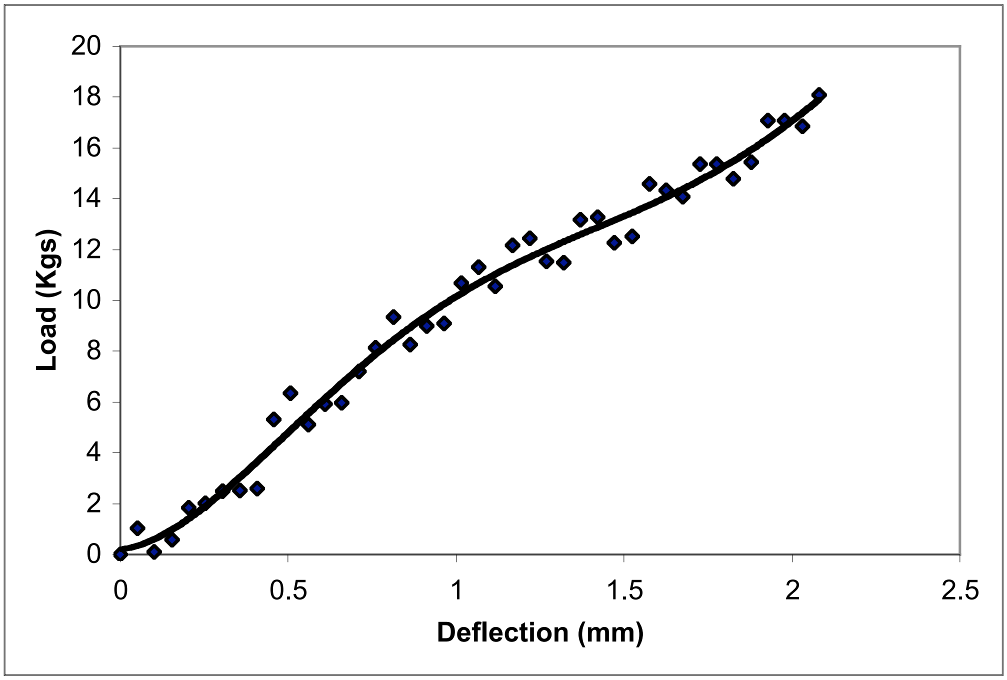

Figure S.3 Load deflection data from a three-point bending characterization test at room temperature (21 ºC) of a square cross-sectional isocyanate-crosslinked, amine-modified silica aerogel ($\rho \sim 0.48$ g cm^{-3}).

Analysis of the load-deflection data of Figure S.3 for deriving the stress-strain curves of Figure 14

Since a material undergoing three-point bending is subjected to both compression at the upper surface and tension at the lower surface, stress (σ) can no longer be calculated by dividing the load by the sample cross section. Instead, stress was calculated using eq S.1, where 'M' is the bending moment and is given by M=PL/4, P is the

$$\sigma = \frac{Mc}{I} \tag{S.1}$$

load applied in the middle of the beam, L is the length of the beam spun, c is the half height of the rectangular beam, and the moment of inertia is given by $I=2bc^3/3$, with b being the thickness of the beam (note that the beam cross-sectional area, A, is thus given by A=2bc). Similarly, normal strain, ε, was determined at the outermost point at the bottom of the specimen via eq S.2, where Young's modulus in flexure (or flexural

$$\varepsilon = \frac{Mc}{EI} \tag{S.2}$$

modulus), E, was determined from the load-deflection relation in three-point bending through consideration of both the bending and the shear energy, which are derived by considering that the three-point bending specimen undergoes both bending as well as shear deformation.[1] Thus, the total strain energy, U (eq S.3) is the sum of the strain

$$U = \frac{P^2L^3}{96EI} + \frac{3P^2L}{5AG} \tag{S.3}$$

energy in bending ($P^2L^3/96EI$) and the strain energy in shear ($3P^2L/5AG$), where G is the shear modulus, and all other symbols have their previously defined meaning. For an isotropic, linear elastic material, G = E/2(1+ν), with ν being the Poisson's ratio. Castigliano's Theorem (eq S.4) relates the load-point deflection (Δ) with the total strain

$$\Delta = \frac{dU}{dP} = \frac{PL^3}{48IE}\left[1 + \frac{48(1+\nu)}{5}\left(\frac{h}{L}\right)^2\right] \tag{S.4}$$

energy,[1] and therefore Young's modulus in flexure (E) was calculated via eq S.5 by

1. Timoshenko, S.; Goodier, J. N. *Theory of Elasticity, Second Edition,* McGraw Hill, New York, 1951, p 147.

$$E = \frac{PL^3}{48I\Delta}\left[1 + \frac{48(1+\nu)}{5}\left(\frac{h}{L}\right)^2\right] \qquad \text{(S.5)}$$

knowing the applied load (P), and measuring the load-point deflection (Δ) directly from the cross-head displacement of the Instron machine. Since there was some variation in the flexural modulus as computed via eq S.5 at various load-point displacements, an average value of flexural modulus was calculated and used in plotting the bending stress-strain data of Figure 14 in the paper.

Movie Index

Movie S.1 Mechanical compression testing of a Desmodour N3200 crosslinked APTES-modified silica aerogel cylinder ~0.5” diameter, ~1” long with ρ~0.48 g cm^{-3}.

Movie S.2 Three-point bending tests on Desmodour N3200 crosslinked APTES-modified silica aerogel rectangular samples with nominal dimensions of 11mm × 11mm × 50 mm (ρ~0.48 g cm^{-3}).