Experimental and Computational Fracture Mechanics

LSU, Feb 2020

Interplay of fracture & plasticity in swelling-driven fracture of phase-transforming battery materials

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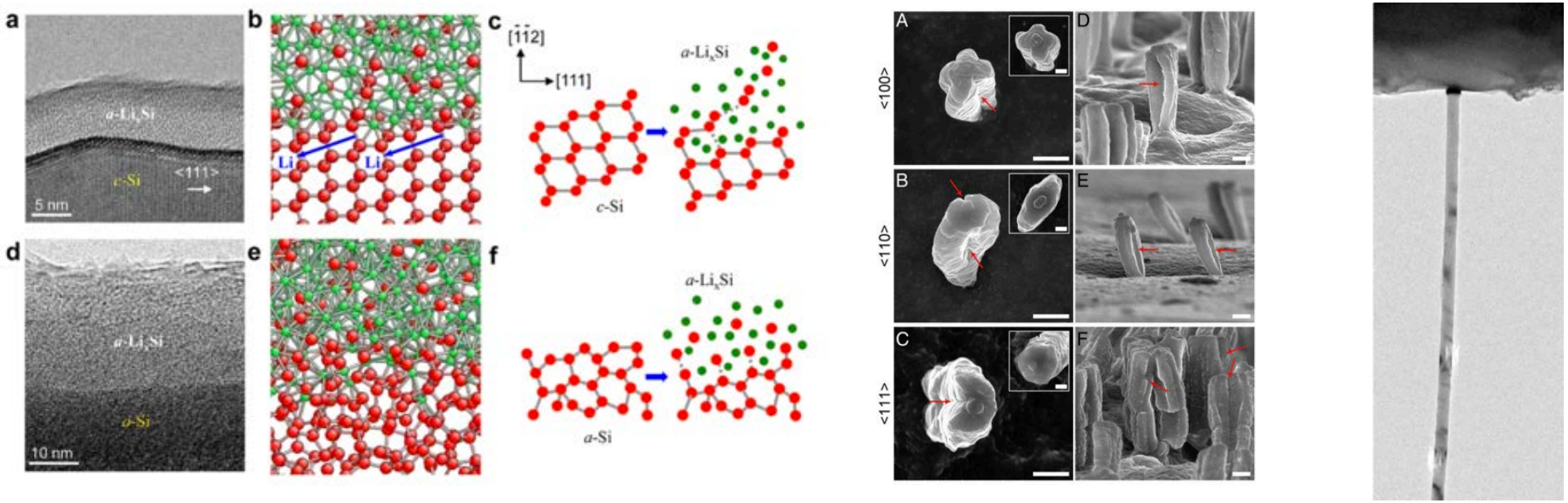
Vulnerable Window of Yield Strength for Swelling-Driven Fracture of Phase-Transforming Battery Materials, A. Mesgarnejad, A. Karma, NPJ Computational Materials 2020

Si phase-change during Li intercalation

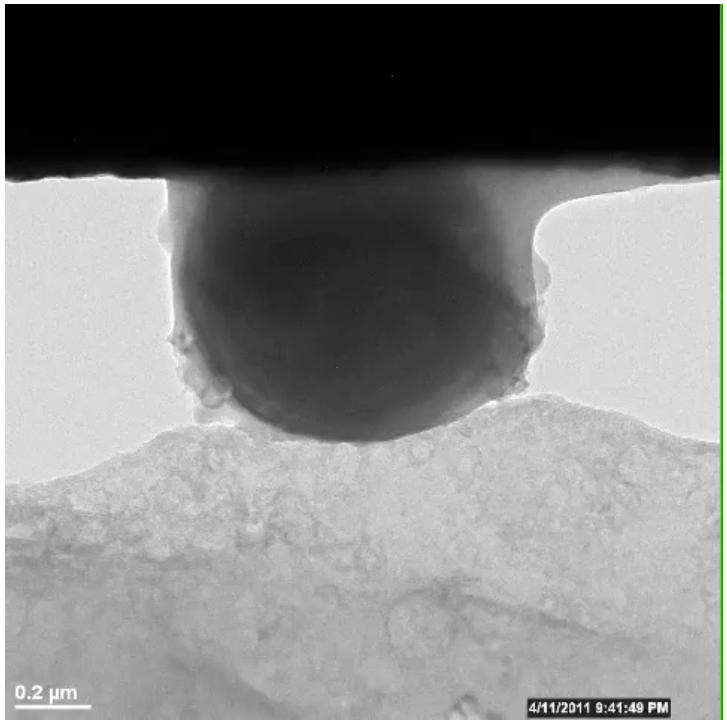


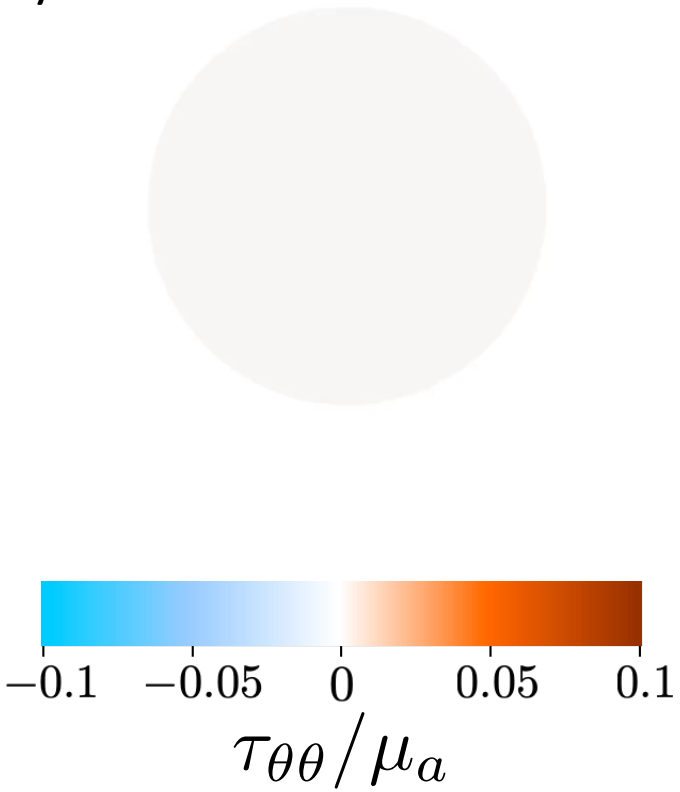
S. W. Lee, M. T. McDowell, L. A. Berla, W. D. Nix, and Y. Cui, Fracture of crystalline silicon nanopillars during electrochemical lithium insertion, Proceedings of the National Academy of Sciences, 109 (2012), pp. 4080–4085.

Liu, X. H., Zheng, H., Zhong, L., Huang, S., Karki, K., Zhang, L. Q., Liu, Y., Kushima, A., Liang, W. T., Wang, J. W., Cho, J.-H., Epstein, E., Dayeh, S. A., Picraux, S. T., Zhu, T., Li, J., Sullivan, J. P., Cumings, J., Wang, C., Mao, S. X., Ye, Z. Z., Zhang, S., and Huang, J. Y. Anisotropic swelling and fracture of silicon nanowires during lithiation. Nano Letters 11, 8 (2011), 3312–3318. PMID: 21707052.

Wang, J. W., He, Y., Fan, F., Liu, X. H., Xia, S., Liu, Y., Harris, C. T., Li, H., Huang, J. Y., Mao, S. X., et al. Two-phase electrochemical lithiation in amorphous silicon. Nano letters 13, 2 (2013), 709–715.

Fracture of a 2D disk:
Nonlinear elasticity without plasticity





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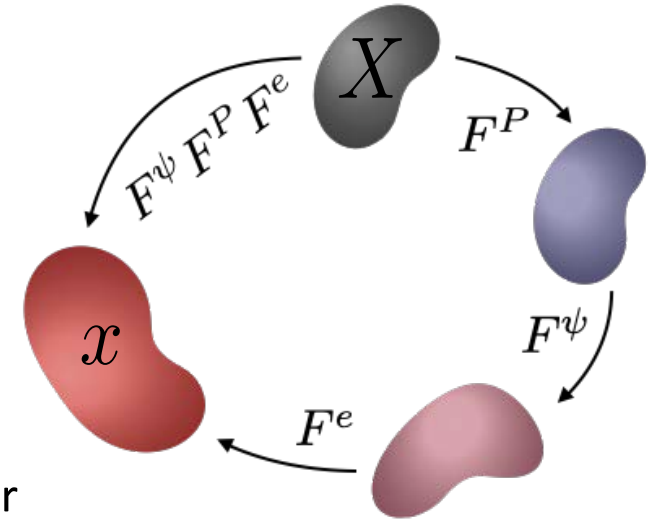
Energy functional

$$E(F^e,\phi,\psi) = \int_\Omega \left(g(\phi)W^+(F^e,\psi) + W^-(F^e,\psi)\right)\, dV$$
$$+\frac{G_c}{4C_\phi}\int_\Omega \left(\frac{w(\phi)}{\xi} + \xi|\nabla\phi|^2\right)\, dV$$
$$+f_0\int_\Omega \left(f_{dw}(\psi) - k f_{tilt}(\psi) + w^2|\nabla\psi|^2\right)\, dV$$

$$g(\phi) = \phi^2 \qquad f_{dw}(\psi) = \frac{1}{4}\psi^2(1-\psi)^2$$

$$w(\phi) = 1-\phi \qquad f_{tilt} = \frac{32}{5}\psi^5 - 16\psi^4 + \frac{32}{3}\psi^3 - \frac{8}{15}$$



Multiplicative decomposition of gradient deformation tensor

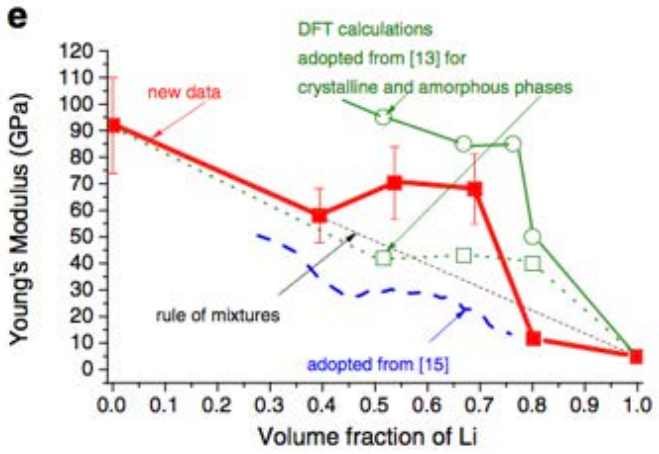
$$F_{ij} = \frac{\partial x_i}{\partial X_j} \qquad I_d + \nabla u = F = F^e F^\psi F^p \qquad F^\psi = (1+\beta\psi)I_d$$

Constitutive equations

Neo-Hookean Elasticity with non-interpenetration

$$\mathcal{W}^{+}(F^e,\psi)=\frac{\mu(\psi)}{2}\left(I_{\hat{C}^e}-N\right)+\frac{\kappa(\psi)}{4}\left(J_e^{+^2}-1-2\ln(J_e^{+})\right)$$

$$\mathcal{W}^{-}(F^e,\psi)=\frac{\kappa(\psi)}{4}\left(J_e^{-^2}-1-2\ln(J_e^{-})\right)$$

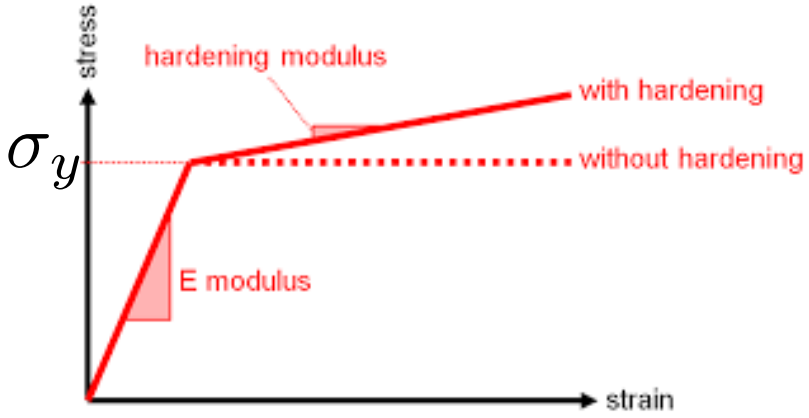


J_2 Plasticity

$$f(\tau,\alpha):=||s||-\sqrt{\tfrac{2}{3}}(\sigma_y(\psi)+K\alpha)\leq 0$$

$$s:=\tau-\frac{Tr(\tau)}{N}$$

$$L_v b^e=-\tfrac{2}{3}\gamma\, Tr(b^e)\frac{s}{||s||}$$



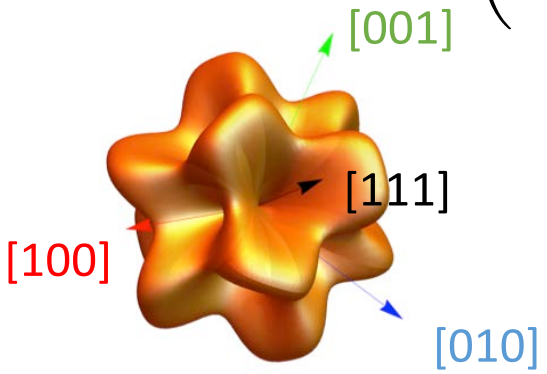
Mobility anisotropy of Li insertion in Si

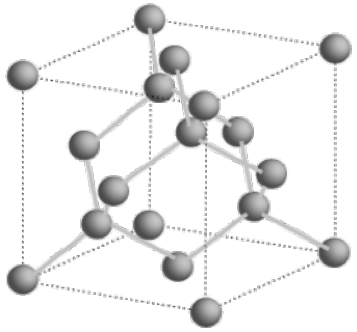
$$x\mathrm{Li}^+ + xe^- + \mathrm{Si} \rightarrow \mathrm{Li}_x\mathrm{Si}$$

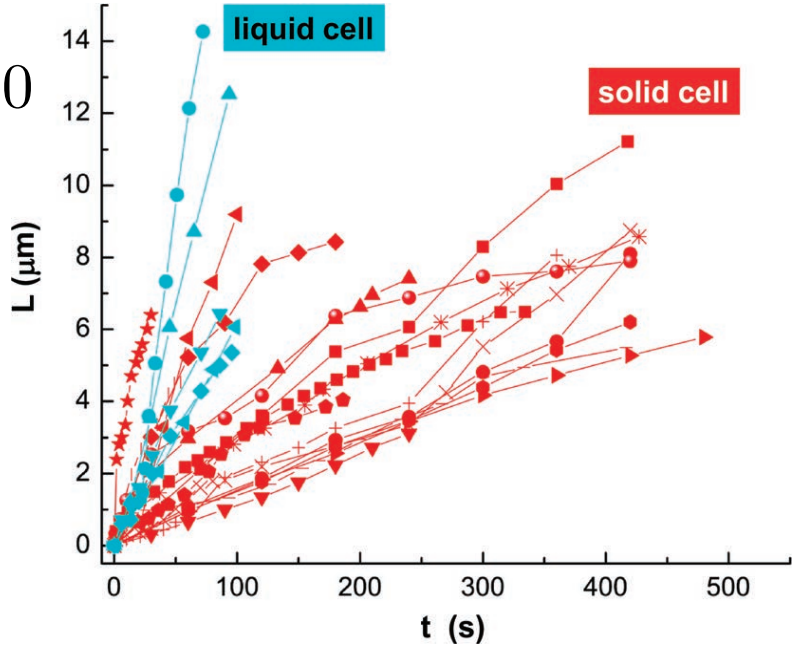
$$\Gamma = x(\tilde{\mu}_{\mathrm{Li}} - \mu^a_{\mathrm{Li}}) + \mu^c_{\mathrm{Si}} - \mu^a_{\mathrm{Si}} - xF\Delta V \geq 0$$

$$V_n = M(\hat{n})\Gamma$$

$$M = 1 - 16(1-\mathcal{A})\left(I_2 - \frac{1}{4}\right)^2 - 3(8+\mathcal{A})I_3$$







Sebastien Nguyen, Roger Folch, Vijay K Verma, Hervé Henry, and Mathis Plapp. Phase-field simulations of viscous fingering in shear-thinning fluids. Physics of Fluids (1994-present), 22(10):103102, 2010.

Liu, X. H., Zheng, H., Zhong, L., Huang, S., Karki, K., Zhang, L. Q., Liu, Y., Kushima, A., Liang, W. T., Wang, J. W., Cho, J.-H., Epstein, E., Dayeh, S. A., Picraux, S. T., Zhu, T., Li, J., Sullivan, J. P., Cumings, J., Wang, C., Mao, S. X., Ye, Z. Z., Zhang, S., and Huang, J. Y. Anisotropic swelling and fracture of silicon nanowires during lithiation. Nano Letters 11, 8 (2011), 3312–3318. PMID: 21707052.