

Abstract Submitted  
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**Modeling the Strength of  $\beta$ -sheet Structures in Silk Crystals and Protein Molecules** DAVID GRUBB, Materials Science & Engineering, Cornell University — The mechanical response of  $\beta$ -sheet structures to a tensile force directed along the axis of one chain can be modeled as an array of elastic springs. The 3-D potential of H-bonds in  $\beta$ -sheets gives a shear stiffness of  $4.5\text{Nm}^{-1}$  and the chain repeat stiffness is  $60\text{Nm}^{-1}$ . Nanocrystals  $>3.5\text{nm}$  long with  $\geq 20$  H-bonds/chain are the strong component of spider silk. They behave much like macro-scale objects, and two conditions must be met for pull-out failure: (1) the load on the most stressed H-bond exceeds the bond strength. (2) the energy of the system is lower after failure. (1) is the critical condition, and the predicted pull-out load is 3-4 times the H-bond strength. An energetically favorable ‘stick-slip’ process is kinetically forbidden. Arrays within a single molecule such as titin have fewer bonds and can fail at low loads by the ‘stick-slip’ process. The logarithmic rate dependence of failure load observed in AFM is  $50\text{pN/decade}$  and the stick-slip prediction is  $30\text{pN/decade}$ . Simulations at short times and high loads give slopes  $>10\times$  higher, matching the prediction for failure at a single bond.

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