Nanoindentation of 35 virus capsids in a molecular model

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A coarse-grained model is used to study the mechanical response of 35 virus capsids of symmetries: T1, T2, T3, pT3, T4, and T7. The model is based on the native structure of the proteins that consitute the capsids and is described in terms of the C$^{\alpha}$ atoms. The number of these atoms ranges between 8 460 (for SPMV -- satellite panicum mosaic virus) and 135 780 (for NBV -- nudaureli virus). Nanoindentation by a broad AFM tip is modeled as compression between two planes: either both flat or one flat and one curved. Plots of the compressive force versus plate separation show a variety of behaviors, but in each case there is an elastic region which extends to a characteristic force F_c. Crossing F_c results in a drop in the force and emergence of irreversibility. Across the 35 capsids studied, both F_c and the elastic constant are observed to vary by a factor of 20. We argue that for a given linear size of the capsid the elastic constant and F_c depend on the average coordination number of an amino acid in the capsid.