A Geometrical Consideration during Forced Stretching of Helical Polypeptides

Atsushi Ikai[1], Rehana Afrin[1,2], Ichiro Takahashi[3] and Kazuki Shiga[3]

[1]Innovation Laboratory, [2]Biofrontier Center, [3]Graduate School of Bioscience and Biotechnology, Tokyo Institute of Technology, 4259 Nagatsuta, Midori-ku, Yokohama 226-8501, Japan
Ikai.a.aa@m.titech.ac.jp

When an alanine based α-helical polypeptide (helicity=70-80%) was stretched from N- and C-termini, a force curve such as given in Fig.1 was obtained [1]. It has an initial gradual increase of force against extension corresponding to stretching of flexible chain followed by a wide region of almost linear increase of the tensile force which is terminated by a sharp force peak representing the rupture of a covalent bond in the system. Events corresponding to the rupture of individual hydrogen bonds were not observed. Instead the tensile force showed a continuous increase almost up to the maximum stretching of the chain when almost no hydrogen bonding was expected.

1. The force curve did not show distinct force peaks corresponding to the breakdown of individual hydrogen bonds in agreement with the theoretical consideration given by Chakrabarti and Levine [2]. They suggested that, since a polypeptide chain with less than 100% helicity is undergoing rapid transition between folded and unfolded conformations, stretching of the chain occurs preferentially at temporarily unfolded local segments because of lower energy barrier and slow experimental time scale. Their prediction for the presence of a plateau in the force curve rather than a constant increase of the force has not been verified yet.

3. The origin of the constantly increasing resistive force was attributed to the presence of an energy barrier between the helical and extended state in the Ramachandran diagram.

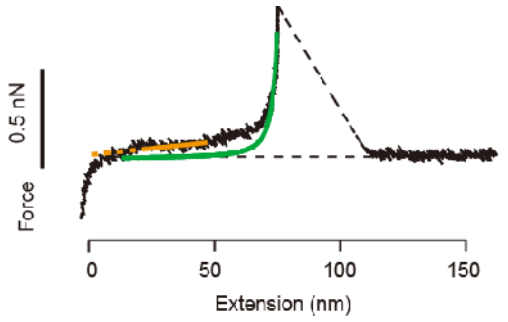

Fig. 1. Experimental stretching curve of alanine based polypeptide from a substantially α-helical to an extended state (dark line) at a speed of ~100 nm/s together with a theoretical curve for an unfolded chain (lowest curve).

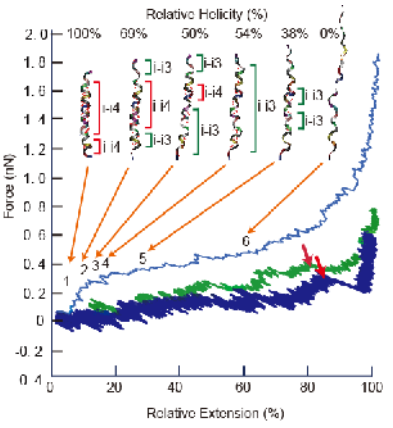

Fig. 2. SMD simulation of α-helix extension at three different speeds 0.1, 0.01, and 0.001 nm/ps from the top line.

References:
1. Afrin *et al.*, 2009. Biophys. J. 96 1105-1114.
2. Chakrabarti *et al.*, 2006. Phys. Rev. E. 74:031903–1 -11.