P.05 Mechanical properties of keratin fibres in complex environments

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Keratin fibres are an important structural component of cells, such as found in skin and nails, that form a cytoskeleton network which gives these cells an elastic response and flexibility.[1] Synthetic keratin films could inspire the development of novel biomaterials where flexibility or shock absorbance could be advantageous. The keratin fibre consists of a hierarchical assembly, starting with the lowest sub-unit; the keratin dimer.[2] While some macro-scale measurements are possible on keratin films and some in vivo fibres, it is very challenging experimentally to isolate and measure the physical properties of an intact dimer, without these denaturing or recombining into the full filament structure.

We have recently attained full atomistic structures of the K1/K10 keratin dimer[3] and are using these as a platform for gaining new insights into the mechanical properties of the fibre.[4] We have performed molecular dynamics simulations of the keratin dimer in its native solvent environment as found in skin – i.e. in the presence of natural moisturizing factors. By changing the environment we have investigated the impact on dimer mechanical properties. In an attempt to connect across the multiple lengthscales of this system and efficiently predict fibre properties, we have determined key energetic and mechanical parameters from the simulations and incorporated them into a mesoscale model of the keratin fibre.

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