Gluten: a fluid or a solid? Insights from coarse-grained molecular dynamics simulations

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Gluten can be obtained by gently washing away soluble components from wheat flour (mostly starch and globular proteins). The remaining mass consists mainly of storage proteins (over 75% mass [1]), which do not seem to have one clearly defined tertiary structure [1], and can form covalently and non-covalently joined complexes in size of megadaltons [2]. This mechanochemical network of gluten proteins is responsible for viscoelastic properties of wheat dough, despite being less than 20% mass of that dough [3]. These properties imply both solid-like behavior (elastic response to deformation) and liquid-like viscous drag from irreversible deformations. These properties can be characterized by dynamic Young modulus $G^* = G' + G''$, which describes response to small-amplitude oscillating deformation: G' for the in-phase (elastic) part and G'' for the out-of-phase (viscous) part. The main goal of this poster is to present a model that can recreate this elastic response of gluten. Existing theories of gluten elasticity point out the crucial role of hydrogen and disulfide bonds between different gluten protein chains [3]. In every gluten protein over 30% of amino acids is glutamine, whose side chain can be both donor and acceptor of hydrogen bonds [3]. This led to the loops-and-trains model [1], which explains gluten elasticity by “loops” created by neighbor polymers: they stay together because of hydrogen bonding, but some bonds are broken (e.g. by water), leading to free space between the polymers (filled by water or other polymers). When polymers are stretched, the free space disappears, and hydrogen bonds reform (causing resistance to further strain). The resistance to stretching is also provided by disulfide bonds that hold some gluten proteins (called glutenins) together, forming a sort of polymer gel [3]. Gluten proteins which do not form inter-chain disulfide bonds (gliadins) are then responsible for the viscous properties of gluten [4]. These theories provide some predictions that can be incorporated into a simple coarse-grained model of gluten. In that model amino acids are represented as pseudoatoms, connected harmonically to form protein chains. Additional interactions include Lenard-Jones potential that mimics hydrogen bonding, and a dynamic potential for disulfide bonds that enables their rupture and reforming. Computer simulations cannot start from the native structure, because of the lack of it, so the chain conformations are generated randomly, and then evolve according to the simplified potential, forming large complexes. Fortunately, local details of structure are not thought to be very important in recreating rheological properties of many interacting polymers [2]. Preliminary results were obtained by periodically deforming the box containing gluten proteins and recording the response force. Amplitude of the force response seems to increase, indicating strain hardening, an effect observed in experiments [5].

[1] P. Shewry, N. Halford, P. Belton and A. Tatham, “The structure and properties of gluten: an elastic protein from wheat grain.” Phil. Trans. R. Soc. B: Biological Sciences, 357(1418): 133-142 (2002).

[2] H. Singh and F. MacRitchie, “Application of Polymer Science to Properties of Gluten.” J. Cereal Sci. 33(3): 231-243 (2001).

[3] H. Wieser, “Chemistry of gluten proteins.” Food Microbiol. 24(2): 115-119 (2007).

[4] R. Kieffer, “The role of gluten elasticity in the baking quality of Wheat.” in The gluten proteins, D. Lafiandra, S. Masci and R. D’Ovidio eds. (Royal Society of Chemistry, Cambridge, 2004).

[5] B. Dobraszczyk, and M. Morgenstern, “Rheology and the breadmaking process.” J. Cereal Sci. 38(3): 229-245 (2003).