Gilberto Igrejas Tatsuya M. Ikeda Carlos Guzmán *Editors*

Wheat Quality For Improving Processing And Human Health



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Preamble

Wheat is one of the most consumed, produced and stored food crops worldwide. The paramount importance of wheat to human populations can be attributed to the remarkable work done by wheat breeders, who have improved wheat varieties keeping them in the spotlight of global agriculture. The recently completed annotation of the entire genome of bread wheat ended 13 years of collective effort to crack the wheat genetic code. The genome sequence can be used to study gene expression at any point in the life cycle of the plant, and to define which genes to target to improve yield and stress resistance. This massive advance not only allowed better understanding of relevant genes for agricultural applications but also for end-use quality traits.

During the last four years, wheat quality scientists from different countries have worked to develop the Expert Working Group (EWG) on Improving Wheat Quality for Processing and Health under the Wheat Initiative umbrella. This joint effort provides a framework to establish strategic research and organisation priorities for wheat improvement at the international level in both developed and developing countries. This EWG aims to maintain and improve wheat quality for processing and health under varying environmental conditions. The EWG has been focused on wheat quality in the broad sense, including seed proteins, carbohydrates, nutritional quality, grain processing and food safety. Bioactive compounds are also being considered, both those with negative effects, such as allergens and mycotoxins, that cause serious problems that need to be resolved, and those with positive effects, such as antioxidants or fibers, that can potentially be exploited. The EWG also works in the development of germplasm sets and other tools that can be deployed in wheat quality research.

The preparation of this book covering the whole range of grain quality topics is one of the important activities that the EWG is doing nowadays. The book should serve to identify possible gaps in important areas of wheat quality research and to position the EWG as an initial point of reference for the global wheat community regarding the different topics covered in depth here. Forty EWG members worked on 21 chapters of the book. This book adheres to the same policies that the EWG promotes such as using unified nomenclature to name the different alleles and providing correct information about materials (accession name, Germplasm Bank of origin, etc.) so other researchers know exactly what is being described and how to obtain the same materials or information.

The present book brings together a group of leading researchers from all over the world who describe different aspects of wheat quality for processing and health. During the meetings of the EWG different topics have been identified in recent years that need close attention or updating so more oriented and ordered research can be carried out in the years to come. The chapters on this topic seek to address this question while capitalizing on outputs of other international initiatives, wheat organizations and other EWGs, namely:

- 1. The importance of wheat
- 2. Wheat gluten protein structure and function: is there anything new under the sun?
- 3. Starch and starch-associated proteins: impacts on wheat grain quality
- 4. Contribution of genetic resources to grain storage protein composition and wheat quality
- 5. Durum wheat storage protein composition and the role of LMW-GS in quality
- 6. Gluten analysis
- 7. Proteomics as a tool in gluten protein research
- 8. Genotypic and environmental effects on wheat technological and nutritional quality
- 9. Improving wheat nutritional quality through biofortification
- 10. Phenolic compounds in wheat kernels: genetic and genomic studies of biosynthesis and regulations
- 11. Wheat cell wall polysaccharides (Dietary Fibre)
- 12. Grain quality in breeding
- 13. High throughput testing of key wheat quality traits in hard red spring wheat breeding programs
- 14. Molecular marker development and application for improving qualities in bread wheat
- 15. Durum wheat products, couscous
- 16. Understanding the mechanics of wheat grain fractionation and the impact of puroindolines on milling and product quality
- 17. The impact of processing on potentially beneficial wheat grain components for human health
- 18. *Fusarium* species infection in wheat: impact on quality and mycotoxin accumulation
- 19. Effects of environmental changes on the allergen content of wheat grain
- 20. Health hazards associated with wheat and gluten consumption in susceptible individuals and status of research on dietary therapies
- 21. FODMAPs in wheat
- 22. Epilogue: The main activities of the International collaboration on wheat quality and safety

In conceiving and compiling this book, we intend to make all these data and recent findings related to the advances on research of wheat quality genomics, proteomics, and other topics accessible to the general scientific community. Considering the importance of this crop in the human diet and its potential to promote health, all the wheat quality research and breeding community will be interested in the topics addressed by the book. Professionals working on the wheat value chain (millers, food manufacturers) or in nutrition and healthcare may also find this book a useful resource to increase and update their knowledge about wheat quality, nutrition and health issues.

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The Importance of Wheat



Gilberto Igrejas and Gérard Branlard

Abstract The history of wheat domestication and use is closely linked to the efforts of humans to protect themselves from hunger and gain control over their food supply. Now grown worldwide wheat has become the most important source of food. For centuries bread wheat (Triticum aestivum) and durum wheat (Triticum durum) have been cultivated in the West to provide humans with energy and essential nutrients. Today China and India are the top two wheat-producing countries, largely because wheat has the advantage of requiring less water for cultivation than other comparable crops while being the main ingredient of a variety of processed foods valued in modern, mainly urban life. For more than a century, breeders have continuously improved wheat focusing on factors affecting grain yield and, more recently, technological quality. The properties of wheat that are ideal for processing into different food products have been greatly improved since the 1960s thanks to detailed research on storage proteins, which constitute the gluten. Most of these genetic successes are referred to in this book but many important goals remain to be achieved. Today further progress is crucial in the use of shared genetic resources, common analytical protocols for allele identification and technological processing, and dedicated tools for analysing polymer formation and characterisation particularly in response to climatic and other environmental factors. Technological properties are not the only wheat quality attributes, as consumers are increasingly aware and concerned about the nutritional value (the content in fiber, minerals, macro- and micro-nutrients, vitamins) and the health impact, whether positive or negative. For example, research on several pathologies associated with the consumption of gluten-based products will require collaboration between allergy specialists and wheat protein geneticists.

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1 Wheat and Humans, a Shared History

Wheat is one of the most important food crops to human populations as it is consumed worldwide. The history of wheat is closely linked to the history of the changing relationship of humans to their environment, and especially the efforts to protect families, tribes and populations from hunger and to master food supply and use. The reader can discover this common past in "The Saga of Wheat" (Bonjean 2016). Long before becoming settled, nomadic peoples ate cereals. Hunter-gatherers would have begun to cultivate the wild emmer (Triticum dicoccoides) 10,000 years BP. Einkorn (Triticum monococcum), the first domesticated wheat (Weiss and Zohary 2011), was cultivated at that time in the Fertile Crescent in a limited area between the Tigris and the Euphrates. Einkorn cultivation appeared in Greece and Balkans around 6000 BC. Later spelt wheat (Triticum *spelta*), and progressively free-threshing wheat (*Triticum turgidum* subsp. *durum*) and hexaploid bread wheat (Triticum aestivum) spread out from the Mediterranean Basin towards eastern, then western Europe, around 4000 and 3500 BC respectively (Bonjean 2016). The spread of wheat to Asia took several routes, including "the steppe route" and "the silk road", around 2500 BC. The Sumerian, Egyptian, Greek and Ancient Roman civilizations gradually came to favour cereal based foods derived from wheat meal and flour (Bruyérin-Champier 1560). The Egyptians taught breadmaking to Greeks, who invented dry yeast and perfected ovens, and after the Persian war Greek prisoners who were bakers would have developed breadmaking in Rome. The Roman Empire took wheat from conquered countries and spread its own culinary habits among the provinces (Flandrin and Montanari 1996). Wheat played such a dominant role in the Roman Empire that it is frequently described as a wheat empire (Shellengerger in Pomeranz 1971). Much earlier in China, the Shang Dynasty (16–11th centuries BC) considered wheat as one of the five sacred plants alongside millet, rice, barley and soybean. Changes in wheat use over the last two millennia clearly shows how people in western countries progressively perfected flour milling, particularly during the industrial revolution in the nineteenth century, as well as flour sieving and mill flow diagrams to get high yielding refined white flour for breadmaking (Branlard and Chiron 2016). These efforts contributed to the rise in the importance of bread wheat for human nutrition compared to other cereals like barley and rye. But the eventual dominance of bread wheat over rye bread was also the result of consumer demand for white bread, the relative increase in wheat production in numerous western countries, the evolution of transport using sea routes and railroad (Braudel 1985), and the improvement in germplasm achieved by agronomists and wheat geneticists. The first hybridizations were developed by de Vilmorin in France from the mid-nineteenth century and by Strampelli in Italy at the beginning of the twentieth century (Bonjean et al. 2011), thanks to the rediscovery of Mendel's laws of genetics.

2 Wheat Yield Improvement

Wheat breeders firstly focused their efforts on characteristics associated to grain yield like lodging resistance, frost resistance, disease resistance of roots, stems and leaves, and grain yield components. World wheat production progressively increased in the twentieth century and particularly after World War II to meet the demands of population growth. Agronomic and genetic advances, particularly through the Green Revolution, made wheat an essential crop to humankind. The total land area given over to bread and durum wheat in the world increased by only 6.8% from 204 Mha to 218 Mha between 1961 and 2013, while world production increased by 321% from 222 MT (a worldwide yield of 1 T/ha) to 713 MT (3.2 T/ha) (FAOstat 2014). Wheat production in 2017 was 757 MT with a harvested area of over 220 M ha, and wheat ranked third in terms of total cereal production behind maize and rice. About 95% of world wheat production is from the hexaploid (*T. aestivum*) bread wheat. According to FAO 2018 figures, China, India and Russia were the top 3 producers in 2017 with respectively 134, 98.5 and 85.9 MT of wheat produced.

3 Wheat Gluten Quality

These remarkable grain yield performances, mainly achieved since the 1960s, were not so successful for quality improvement. At the beginning of the twentieth century, the only measure breeders could use to assess grain quality was the Kjeldahl assay for nitrogen content. Several empirical tools were designed, like the Extensograph, Alveograph, Mixograph, and Farinograph, to indirectly test grain quality by measuring flour and dough properties and these were adopted for use in breeding programs to follow and select quality traits (Branlard and Chiron 2016). Breadmaking quality, which combines several characteristics like rheological dough properties, dough fermentation, gas retention, crumb texture, loaf volume, crust color, is highly polygenic and of low heritability. Moderate progress was made in genetic improvement of cultivars after the 1950s using indirect tests. Since the 1980s, progress accelerated thanks to the breakthroughs resulting from genetic analysis of wheat storage proteins, the components of gluten (Biesiekierski 2017).

The processing properties of wheat are largely determined by gluten proteins. Beccari was the first to successfully isolate gluten proteins around the mideighteenth century (Bailey 1941). Thomas Osborne (1907) later classified grain storage proteins based on their solubility. Albumins are water soluble, globulins are salt soluble, prolamins are soluble in aqueous ethanol and glutenins remain in the flour residue. Storage proteins became the focus of many studies and biochemical, genetic and molecular approaches greatly helped to decipher the major roles played by glutenins and gliadins in determining gluten properties. These proteins form a complex network during dough processing, giving the unique property of viscoelasticity to the dough. Different types of food can be made depending on the particular balance of functional properties of the dough, because the relative composition and variations in glutenins and gliadins have important effects on gluten behaviour (Wang et al. 2017). Since 1980 thirteen International Gluten Workshops have been held around the world acting as milestones that show the great progress achieved in all aspects of gluten research for bread and durum wheat uses. For instance, the gluten proteins were among the first genetic markers employed in breeding for bread wheat and durum wheat quality.

4 Wheat for Industrial Uses

Industry has developed specific processes for starch extraction from corn and wheat. Modern manufacturing plants can extract 40–50 T of flour per hour in a low water input centrifugation process. More than 30 countries today have private wheat starch industries but publicly available statistics are rather scarce. Several hundred products are currently prepared from wheat starch like:

- Food additives like sweetener in beverages, binding agent in soups and sauces, moistening agent in bakery, texture agent in many dairy products, etc.
- Green chemistry (fermentation), adhesives, bioplastics, paper industry, ethanol etc.
- Baby food, energy drinks, emulsifier, etc.
- Animal feed (milk powder), piglet starter feed, aquaculture feed pellets, etc.

The wheat starch industry generates a "first-class byproduct", gluten. The increase in wheat starch production worldwide has made gluten the cheapest "green protein" now available for any food or feed producer.

In developed countries millers have turned to adding gluten powder to flour to improve the rheological and technological properties to the levels required by the baking industry. Between 0.2% and 10% of gluten can be added to flour according to the characteristics sought for the numerous food products that can be made like steamed buns, toast breads, crusty breads, sweet breads, leavened and laminated sweet goods, laminated puff pastries, rolls and buns, crackers, cookies, sponge cakes, wafers, and snacks (Branlard and Chiron 2016). These products are much more compatible with the "western lifestyle" as they are easily produced and consumed, making them preferable to the traditional ones (Shewry and Hey 2015). Wheat gluten is also largely used as a protein binder in a variety of food preparations like for meat mixes in sausages.

For the feed industry, the gluten now available can be used in a variety of ways. Gluten's insolubility in water and its binding properties are an advantage in aquaculture in reducing pellet breakdown and providing fish with 'green' proteins. Gluten is also used in the preparation of biopolymers, in which the genetic diversity of glutenin can be exploited to tailor specific polymers (Johansson et al. 2013).

Wheat is also used for animal feedstuff, mainly for poultry diets (Bushuk and Rasper 1994). The European Common Agricultural Policy greatly helped this

development by granting premium for cereals incorporated into feedstuffs. As an example, each year around 12% of wheat produced in France is incorporated into feedstuffs. This usage as a feed grain is directly dependent on the price relationship between wheat and other crops meaning that in years where harvests are negatively affected by climatic conditions and there is excess grain unsuitable for human consumption, this will be used to feed livestock. Other uses of low-grade grain are in the production of alcohol, adhesives, paper additives, soaps, rubbers, cosmetics and varnishes, the wide range of uses contributing to its increasing demand and production (Peña-Bautista et al. 2017). More transparency may be necessary to inform customers and consumers of the myriad products which contain ingredients derived from wheat.

5 Important Questions to Be Addressed

The diversity of storage proteins remains a central aspect to study for the decades ahead. To further our understanding of gluten properties, international cooperation on the following topics related to storage proteins will be of prime importance for geneticists, breeders, scientists and nutritionists interested in wheat quality. (1) Wheat genetic resources must be managed such that any known cultivars with specific allelic compositions are made available to the community of scientists. (2) The analytical protocols for allele identification and nomenclature (using electrophoresis, chromatography, DNA sequencing or proteomics tools) and for technological properties assessment have to be shared among the scientific community to ensure comparability of results. (3) Molecular mechanisms involved in the polymerization of storage proteins in protein bodies need to be elucidated. Specific tools for analysing polymer characteristics (mass, size, dispersity index), particularly to measure responses to climatic and environmental factors, will need to be used.

Wheat storage proteins are also responsible for celiac disease as they trigger an immune response when eaten by susceptible individuals leading to inflammation and small intestine damage (prevalence 1-3%), and are associated to several pathologies like wheat dependent exercise-induced anaphylaxis, an immediate hypersensitivity (prevalence <0.1%) (Laurière et al. 2007). A recent health trouble (Alessio et al., 2015) has been attributed to gluten, non-celiac gluten sensitivity (NCGS), the prevalence of which could be up to 6% in the US population (Igbinedion et al. 2017). Candidate proteins responsible for NCGS are actively sought. Amylase-trypsin inhibitors (ATIs) known to be nutritional activators of innate immunity and resistant to proteases could be possible candidates as they have been shown to increase intestinal inflammation (Zevallos et al. 2017). It is worth pointing out here that the characteristics of polymers are largely influenced by high temperature during storage protein accumulation in the grain, but this aspect has yet to be investigated in relation to the human pathologies (Branlard et al. 2019a, b).

Wheat grain is today the most important source of food on earth. It contains 75–80% carbohydrates, 9–18% protein, fiber, many vitamins (especially B

vitamins), calcium, iron and many macro- and micro-nutrients. Heritability estimates of the content of several vitamins and nutritional constituents, including arabinoxylans, have shown that there is potentially useful genetic variability that can be exploited in breeding new varieties (Saulnier et al. 2007, Shewry et al. 2012). The importance of wheat for human nutrition and health is not sufficiently prioritized today by breeders and nutritionists. The recently completed annotation of the entire complex bread wheat genome (15,961 megabases) ended 13 years of collective effort from multiple researchers to crack the genetic code of this cereal. This massive step forward will not only improve our understanding of the role of relevant genes throughout plant development, but also, combined with proteomics and metabolomics, help to target end-use quality traits and valuable wheat grain components for better nutrition and health.

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Wheat Gluten Protein Structure and Function: Is There Anything New under the Sun?



Ramune Kuktaite and Catherine Ravel

Abstract This chapter focuses on wheat gluten protein and how its protein components, gliadin and glutenin, interact at the molecular level to produce structures, which contribute to particular functional properties. The aspects of gluten protein are highlighted in wheat gluten, in both, food and non-food products. Factors impacting wheat gluten protein chemistry and structure under various processing conditions and in different end-use products are discussed. The influence of the genetic make-up of wheat grain on the molecular structure and functional performance of gluten protein in the end-use products is discussed. The main factors steering wheat gluten protein structure-function relationships are thus summarised in the context of traditional and innovative applications.

1 Introduction

Wheat (*Triticum aestivum* L.), cultivated at latitudes spanning from Scandinavia to Argentina, is one of the most widely grown crops in the world. Around 90% of wheat is used for human consumption in various its forms such as, bread, cookies and pasta etc. Therefore, the most important aspects of wheat grain quality are the nutritional value due to the grain bioactive components, dietary fibers, minerals and vitamins, notably B vitamins (Hussain et al. 2012a, 2012b, 2012d, Shewry and Hey, 2015) and its breadmaking quality characteristics, such as milling, processing and baking performance (Hernandez-Espinosa et al. 2018; Guzman et al. 2015). The remaining 10% is used as seed or flour for industrial production of gluten, starch and other products. The major factors determining the quality of processed wheat food products are grain storage protein (about 80% of the grain total protein) content

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and composition (Shewry et al. 2002). These proteins are able to interact with each other and form the proteinaceous network when the wheat flour is mixed with water. The gluten protein fraction impacts the end-use quality of wheat-derived foods in specific ways. These proteins have also recently been evaluated for their applicability in innovative non-food materials, such as bio-based plastics (Rasheed et al. 2015, 2016; Johansson et al. 2013; Kuktaite et al. 2011). The physicochemical, structural and functional properties of processed wheat gluten products are to a large extent determined by the presence and proportions of gliadins and glutenins and the molecular interactions they foster through disulfide bonds and non-covalent Van de Waals forces, as well as through hydrogen and isopeptide bonds (Rombouts et al. 2013; Rasheed et al. 2018; Kuktaite et al. 2004). Many factors are known to contribute to the structural and functional properties of gluten protein during processing, as for example in dough. When wheat dough is mixed for an optimum time, more structurally ordered, homogeneous and elastic gluten is formed (Kuktaite et al. 2004). Different structure-function relationships are observed in dough produced from different wheat varieties (Shewry et al. 2001). In the processing of bio-based plastics from gluten, hierarchical structures are formed in the presence of specific additives or when specific conditions are applied (Kuktaite et al. 2011, Johansson et al. 2013; Muneer et al. 2015; Türe et al. 2011). The genetic composition of wheat gluten protein also has an impact (Rasheed et al. 2016). The characteristic properties of gluten, particularly viscoelasticity and extensibility, in relation to the structures formed in the processing of diverse wheat products are very important and have been the focus of basic and applied research for more than 260 years (Wieser and Kieffer 2001). Then how can wheat gluten structures and properties be finetuned to modify and improve end-use quality of wheat products in all their diversity? Understanding more about the basis of wheat gluten functionality is directly relevant to optimize gluten processing in various industrial applications, and could be used by breeders to improve wheat varieties suited to desired end-use requirements. This chapter summarizes some of the latest studies of food and non-food gluten systems to review the factors influencing the structure-function relationships of wheat gluten and includes genetics, chemistry, structure and processing technology.

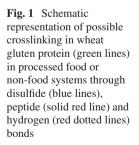
2 Wheat Grain Proteins Are Key Factors for Functionality of Wheat Flour Processing to Food and Non-food Products

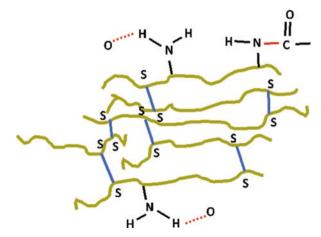
Wheat grain proteins are divided into functional proteins (albumins, globulins) and grain storage proteins that provide nutrients such as amino acids to the growing plant (Day et al. 2006). Grain storage proteins also called prolamins consist of monomeric gliadins and polymeric glutenins. Gluten protein are known for their impressive level of diversity. Gliadin proteins are divided into the four main types α -, β -, γ - and ω -gliadins according to their electrophoretic mobility in acid condi-

tions, the α - and β -gliadins being closely related in terms of structure. Glutenins are either high molecular weight (HMW) or low molecular weight (LMW) types. The β -spiral structure of HMW glutenins explains their intrinsic elasticity (Shewry et al. 2001). As sulfur plays a special role, they are also divided into groups that differ by their S-amino acid composition (Shewry et al. 2001). S-rich gluten proteins consist of α/β - and γ -gliadins and LMW glutenins. S-poor gluten proteins correspond to ω -gliadins and HMW glutenins.

The gluten confers special characteristics to bread made from the common wheat (*Triticum aestivum* L.) flour (Shewry et al. 2002), to pasta made from durum wheat flour (*Triticum turgidum* L. var. *durum*) and to bio-plastics made from industrially produced gluten after starch has been removed (Rasheed et al. 2015). The gluten proteins have unique viscoelastic properties, which are distinct from their structural and functional aspects. Roughly, glutenins confer the gluten elasticity and tenacity while gliadins confer viscosity (MacRitchie 1999; Shewry et al. 2002). Gluten proteins can easily polymerize and form large complex polymers with low solubility, which hampers research efforts to determine their structures. Despite this, several studies have proposed some interpretations of the structure-function relationships of gluten, where HMW glutenins and LMW glutenins interact *via* disulfide and other types of bonding to form its backbone. The formation of disulfide bonds and their interchange reactions, as well as non-covalent Van der Waals interactions have been well studied in gluten food systems (Belton 1999; Wieser 2007).

When gluten is used for non-food applications such as bioplastics, films, or foams, and it has clearly been shown that the molecular organization of the protein includes disulfide crosslinks, hydrogen bonding, as well as non-reducible isopeptide bonding, and lanthionine and lysinoalanine interactions (Rombouts et al. 2010, 2013; Kuktaite et al. 2016; Blomfeldt et al. 2011; Türe et al. 2011) (Fig. 1). The characteristics and end-uses of both food and non-food wheat gluten products mainly depend on gluten strength. Therefore improving gluten strength and protein





content in the grain have been emphasized as among the most important targets in breeding of different types of wheat (Shewry et al. 2002; Patil et al. 2009).

There are significant challenges in the wheat sector arising from a growing demand for food driven by the world's growing population, rapidly changing food preferences, and challenging climate variation and the need for healthier food to improve diet and combat diseases. In addition, wheat protein provides about 20% of the total protein in the human diet. Therefore, wheat protein could play an important role towards a more sustainable alimentation with a smaller part of animal protein. The production of this higher quality wheat must also take into account concerns over the impact on agricultural systems and on the environment, as well as the effect of climate change on the stability of wheat quality. Most of these concerns require wheat with a specific quality profile in terms of protein concentration and composition, which mainly define gluten strength that is most closely suited to its intended end-use.

In conclusion, wheat quality is a very complex characteristic to deal with and depends on many parameters as grain yield because it is negatively correlated to protein concentration. Similarly genetically determined protein composition (Malik et al. 2013) also influence this trait, and for end-use value, several studies have ranked gliadin or glutenin alleles in order of their influence on flour quality as decribed in the pionner studies of Branlard and Dardevet (1985) or Payne in 1987. Wheat grain quality directly impacts mixed dough (Kuktaite et al. 2004, 2005) and end-product such as, bread quality (Hussain et al. 2012b, 2012c, 2013).

3 Wheat Gluten Protein Structure During Processing

3.1 Impact in Food Processing

Wheat gluten proteins in the presence of water form a viscoleastic protein network and with the starch in dough can produce structures suitable for various end-uses. The importance of the viscoleastic properties of wheat dough in breadmaking and other wheat product processes have been well described (Shewry et al. 2002). Thermal polymerization of gliadins and glutenins occurs, for example, during bread baking or pasta making processes, and is related to the formation of covalent bonds between polypeptides or different parts of a polypeptide (Lagrain et al. 2007; Cubadda et al. 2007). Gliadins and glutenins under alkaline conditions are known to form unreducible covalent crosslinks, such as those formed through lanthionine or lysinoalanine (Rombouts et al. 2010). Isopeptide bond formation involving glutamine residues and heat treatment has been suggested to occur in bread, pasta and gluten films (Sakamoto et al. 1995; Petitot et al. 2009; Rombouts et al. 2013).

Baking quality is usually determined through a number of tests, including dough rheology and mixing tests that assess the viscosity and elasticity during dough preparation, together with complex tests of extensibility and baking (Guzman et al. 2015, Wang and Kovacs 2002; Li et al. 2015). Mixing behaviour, including parameters

such as the optimal mixing time to form a gluten network, has been found to impact the gluten structure and rheological behaviour of the resultant dough (Kuktaite et al. 2005). However, performing all these tests is time consuming and expensive. The genetic determination of baking quality of flour and dough have been studied (Bordes et al. 2011) and some molecular markers could be used to improve quality. On another hand, genomic selection could be used to predict quality traits by taking into account the effect of a large number of markers (Meuwissen et al. 2001) as was done in a recent research attempts by Guzman et al. (2016a). For example, CIMMYT has used genomic selection to predict all of the processing and end-use quality traits in the spring wheat breeding program (Guzman et al. 2016b) while Michel et al. (2018) has used this method to improve baking quality.

3.2 Impact in Non-Food Processing

The unique properties of wheat gluten in forming polymeric protein matrices made it an interesting subject of applied studies in the area of bioplastics (Kuktaite et al. 2011; Türe et al. 2011; Blomfeldt et al. 2011; Rasheed et al. 2015). Another reason for growing interest in wheat gluten protein is the worldwide move to replace synthetic plastics with polymers from renewable agro-resources as a solution to pollution caused by non-biodegradable synthetic polymers (Payne and Corfield 1979). In addition, gluten is a cheap product from starch industries, which search outlets for this sub-product. Previous studies have revealed the importance of key parameters such as genetic make-up and cultivation inputs to the plant (Rasheed et al. 2015; 2016), as well as chemical and physical treatments of gluten protein during processing. The latter treatments applied to gluten were used in making films, foams and composite forming materials, respectively (Kuktaite et al. 2012, 2014; Muneer et al. 2015, 2016; Rasheed et al. 2014; Johansson et al. 2013). The reactive chemistry of gluten originates from the available modifiable protein side groups, which make it possible to obtain three-dimensional polymeric protein networks with appropriate strengths and functional properties (Yu et al. 2016; Kuktaite et al. 2011, 2014, 2016; Andrade et al. 2018; Rasheed et al. 2016). Processing methods such as solution casting and foaming, including those related to temperature and pressure conditions like extrusion and compression molding, have been widely used to process gluten (Gontard et al. 1992; Gennadios et al. 1993; Kuktaite et al. 2011, 2012, 2014, 2016). In various studies, aggregation or pre-aggregation of gluten proteins was observed to take place at earlier stages of processing. Crosslinking between gluten protein molecules through disulfide/sulfydryl interchange reactions, hydrophobic interactions and iso-peptide bonding occurs according to the chosen temperature, additives used or processing method. The protein secondary structures, and the micro- and nano-structures in gluten, gliadins and glutenins, processed alone or with starch are summarised in Table 1.

Wheat gluten protein structure formation at various molecular levels (from macro through micro to nano) has been correlated with functional properties in a

Protein type and processing conditions	Secondary structure	Microstructure	Molecular distances d, Å
Wheat gluten Gluten blend with modified potato starch, temperature (plasticizer)			SAXS data from Muneer et al. 2015
Protein:starch ratio 30:70, 110 ° C (glycerol)			$d_1 = 89.4, d_2 = 55, d_3 = 16.2$
Protein:starch ratio 50:50, 110 ° C (glycerol)			$d_1 = 85.5, d_2 = 55, d_3 = 16.1$
Protein:starch ratio 70:30, 110 ° C (glycerol) Protein:starch ratio 30:70, 130 ° C (glycerol) Protein:starch ratio 50:50, 130 ° C (glycerol) Protein:starch ratio 70:30, 130 ° C (glycerol) Protein:starch ratio 50:50, 110 ° C (water + glycerol) Protein:starch ratio 50:50, 130 ° C (water + glycerol)	β-sheets β-sheets	non- homogeneous homogeneous	
Gliadin			SAXS data from Muneer et al. 2016
Gliadin only, 110 ° C (glycerol) Gliadin:starch ratio 30:70, 110 ° C (glycerol) Gliadin:starch ratio 50:50, 110 ° C (glycerol) Gliadin:starch ratio 70:30, 110 ° C (glycerol) Gliadin only, 130 ° C (glycerol) Gliadin:starch ratio 30:70, 130 ° C (glycerol) Gliadin:starch ratio 50:50, 130 ° C (glycerol) Gliadin:starch ratio 70:30, 130 ° C (glycerol) Gliadin:starch ratio 70:30, 130 ° C (glycerol) Gliadin:starch ratio 70:30, 130 ° C (glycerol)	β-turns, $β$ -sheets and unordered β-sheets, weak $β$ -sheet interactions, $β$ -turns β-sheets, weak $β$ -sheet interactions, $β$ -turns β-turns, $β$ -sheets and unordered β-turns, $β$ -sheets and weak $β$ -sheet interactions weak $β$ -sheet interactions, $α$ -helix & random coil, $β$ -turns	non- homogeneous	$\begin{array}{l} d_{broad} = 106.7, d_1 = 55.9\\ d_2 = 32.3, d_3 = 28.1\\ d_{broad} = 94.6, d_1 = 57.9,\\ d_2 = 33.6, d_3 = 29.2\\ d_{broad} = 92.1, d_1 = 57.3,\\ d_2 = 33.2, d_3 = 28.8\\ d_{broad} = 96.3,\\ d_1 = 56.6, d_2 = 32.8,\\ d_3 = 28.4\\ d_{broad} = 97.1, d_1 = 56.1,\\ d_2 = 32.5, d_3 = 28.2\\ d_{broad} = 93.8, d_1 = 58.2,\\ d_2 = 33.8, d_3 = 29.3\\ d_{broad} = 99.2, d_1 = 59.3,\\ d_2 = 34.4, d_3 = 29.8\\ d_{broad} = 96.6, d_1 = 57.9,\\ d_2 = 33.7, d_3 = 29.2\\ \hline \emph{WAXS \ data} \end{array}$
			<i>from</i> Rasheed et al. 2018
Genotype 2 + 12, A* Genotype 5 + 10, B**	strong β -sheet interactions, α -helices & random coils, β -turns strong β -sheet interactions, α -helices & random coils, β -turns		$\begin{array}{l} d_1 = 6.8, d_2 = 4.5, \\ d_3 = 3.9, d_4 = 2.7, \\ d_A = 9.6 \\ d_1 = 6.8, d_2 = 4.5, \\ d_3 = 3.9, d_4 = 2.7, \\ d_A = 9.7 \end{array}$

 Table 1
 Wheat gluten structures observed in different non-food systems.

SAXS, small angle X-ray scattering. WAXS, wide-angle X-ray scattering.

A* and B** refer to growing environments from Rasheed et al. 2018

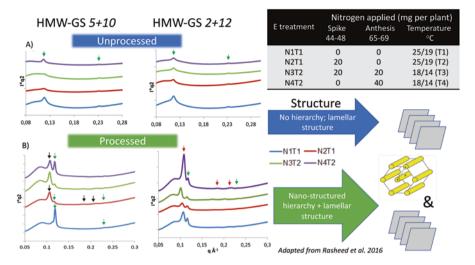


Fig. 2 Wheat gluten protein nanostructure studied by small-angle X-ray scattering. Gluten was extracted from wheat lines with genetically different HMW glutenin compositions (HMW-GS 5 + 10 and HMW-GS 2 + 12) grown in 4 different environments as specified in the table (insert). Variation in nanostructural profiles of (A) unprocessed and (B) processed gluten showing the detection of lamellar (small green arrows) and hexagonal structural arrangements (red arrows) shown schematically in diagrams (bottom right). Modified from Rasheed et al. 2016

number of studies (Kuktaite et al. 2011, 2014, 2016; Muneer et al. 2015, 2016; Rasheed et al. 2014, 2016, 2018; Johansson et al. 2013; Andrade et al. 2018). In particular, the formation of hierarchically arranged nano-structures of gluten proteins (Kuktaite et al. 2011) or complex hierarchical hexagonal and lamellar structures can be highlighted (Fig. 2, modified from Rasheed et al. 2016). The formation of hexagonal structures was also observed in gliadins that had been temperature processed in a blend with glycerol (Kuktaite et al. 2016; Muneer et al. 2016).

4 Structure-Function Relationships in End-Products from Processed Wheat

Being able to combine genetic, structural and functional information into a model that can predict end-use characteristics of processed wheat gluten protein is still a valid goal. Some attempts to correlate the molecular structure of gluten protein with the mechanical behavior of bio-based materials have been made. Crosslinking, structure and baking performance in baked wheat products, such as bread, have been broadly studied, but more research is needed to account for other factors such as genetics, growing environment, and structure-function relationships. By extracting gluten in mild conditions, it is foreseeable that genotypes could be selected based on the strong mechanical performance of non-food gluten material (Rasheed et al. 2018). The potential for a broad range of qualities for non-food gluten materials should be further explored. For prediction of wheat bread baking performance, methods to screen for quality including structural characteristics and functional behavior should also be further improved.

5 Conclusions and Summary

The use of multiscale and multistage factors, including genomic selection, to assist in the assessment and prediction of wheat quality, as well as the prediction of all of the processing and end-use quality traits in wheat is a priority. In this context, a good understanding of the relationship between gluten structure and function is needed to tailor wheat gluten proteins to specific food and non-food end-uses.

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Starch and Starch-Associated Proteins: Impacts on Wheat Grain Quality



Ahmed Regina and Carlos Guzmán

Abstract Wheat storage proteins have been historically examined and periodically established to be the major determinant of wheat quality. Gluten proteins largely contribute to the formation of viscoelastic network in a dough, enabling processing of wheat to food products including bread. More recently starch, the major component constituting 60-70% of wheat grain, is understood to play key roles in flour quality, dough functionality and end product and nutritional quality. Starch is composed of two neutral macromolecules of glucose, amylose and amylopectin. The structural differences between amylose and amylopectin are predominantly dependent on the extent and distribution of α -1,4 and α -1,6 linkages that connect the glucose units to form these two polymers. The functional properties of starch as governed by its structure, molecular organisation, granule morphology and size distribution influence dough behaviour during processing, differentially impacting the end product qualities. Also, varyingly important are the roles of starch granule associated proteins, comprised of both surface proteins and granule-integral proteins with enzyme functions, in driving starch responses in a complex dough matrix system. This chapter aims to provide an extensive review on how starch, associated proteins and starch-protein interactions influence functional properties of food systems.

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