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# Decoding the glass genome

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ABSTRACT

Glasses have played a critical role in the development of modern civilization and will continue to bring new solutions to global challenges from energy and the environment to healthcare and information/communication technology. To meet the accelerated pace of modern technology delivery, a more sophisticated approach to the design of advanced glass chemistries must be developed to enable faster, cheaper, and better research and development of new glass compositions for future applications. In the spirit of the U.S. Materials Genome Initiative, here we describe an approach for designing new glasses based on a mathematical optimization of composition-dependent glass property models. The models combine known physical insights regarding glass composition-property relationships together with data-driven approaches including machine learning techniques. Using such a combination of physical and empirical modeling approaches, we seek to decode the "glass genome," enabling the improved and accelerated design of new glassy materials.



## 1. Introduction

Throughout human history, glass has been one of the most vital and influential of all materials, and the importance of glass is only growing [1]. While often taken for granted, glass windows enable visible light into buildings and vehicles while sheltering the occupants from harsh weather conditions [2]. Modern high-tech glasses, such as photochromic [3] and electrochromic [4] windows, can dynamically adapt to sunlight conditions to improve energy efficiency for applications in architecture and transportation. Moreover, the use of thinner, lightweight strengthened glass can improve fuel economy in vehicles without compromising safety [5].

In addition to glass windows, the development of glass lenses is another society-changing invention that has brought the world into focus for people suffering from vision problems. Glass lenses were also the essential invention for revolutionizing the field of astronomy and for enabling the discovery of microbiology [6]. Today, glass lenses are ubiquitous in computers and other personal electronic devices.

The invention of low-loss glass optical fibers was key in the development of the Internet, enabling exponentially growing levels of communication across the globe [7]. Glass has also played a revolutionary role in the display of information, from early televisions based on cathode ray tubes to modern flat panel displays [8]. As the resolution of these displays improves, the requirements on the high-tech glass substrates have become tighter and tighter [9]. New glasses will also be key for visualizing information through augmented and virtual reality devices.

Strengthened glasses with high chemical durability have been critical for healthcare applications such as pharmaceutical packaging [10]. Within the realm of healthcare, bioactive glasses have also been developed to address a wide range of medical problems, including bone repair, cancer therapy, soft tissue repair, and dental applications [11].

Owing to these many highly impactful applications of glass—addressing major global challenges in energy, communications, healthcare, information display, safety, and more—an argument has been made that we are now living in the Glass Age [12]. However, the current applications of glass represent only the beginning of what this versatile class of materials will offer.

Future applications necessitate the careful design of new glass compositions to meet stringent requirements for both product attributes and the properties required for large-scale manufacturing. To accelerate the design of new glassy materials, it is imperative that we make comprehensive use of available modeling tools [13]. The concept of the "materials genome" was first conceived by Prof. Zi-Kui Liu at the Pennsylvania State University [14] and then independently by Prof. Gerband Ceder and coworkers at MIT in the 2000s [15,16]. The concept borrows from the idea of biological genomics, which involves the sequencing and analysis of the genomes of living organisms, with the overall goal of connecting the observable characteristics of the organisms with their underlying genetic chemistry. The concept of the materials gen-

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ome is analogous to biological genomics, but applied in the field of materials science and engineering. In this case, the goal is to make quantitatively accurate predictions of material properties based on their underlying chemical makeup. For our current work, we use a combination of both physics-based and empirical models to help elucidate the origin of glass properties and pave the way toward composition optimization for emerging applications. By developing models for each property of interest, we can decode the "glass genome" to enable the design of new transformative materials to meet many of the grand challenges faced by the world today and in the future.

## 2. Glass design considerations

One of the defining characteristics of glass is its non-crystalline structure, lacking the long-range atomic ordering found in crystalline materials. Owing to this non-crystalline structure, a glass does not need to satisfy the same stoichiometric requirements as in crystal chemistry [17]. Coupled with the fact that nearly every element of the periodic table can conceivably be incorporated into a glass, there are an essentially infinite number of potential glass chemistries available. Since the composition of a glass can be continuously adjustable, glass properties can be fine-tuned, potentially down to an atomic level of precision. When designing new glass compositions, it can therefore be daunting to consider the extraordinary number of possible glass chemistries [18]. But, as indicated in Fig. 1, this is also an excellent opportunity to make use of predictive modeling tools to accelerate the design and optimization of new glassy materials.

The design of new glass compositions involves a balancing of different product- and manufacturing-related attributes, such as the examples shown in Fig. 2. Product-related attributes include any property of the material that is required to achieve the desired product performance. To be a successful product, the glass must meet all of these property requirements and exceed the performance of other competing products. Relevant attributes depend on the application of the glass and often include mechanical, chemical, thermal, optical, and dynamic properties [13].

Successfully achieving product-related properties is only half of the story. We must also ensure that the glass can be successfully manufactured at a scale required to meet customer demand. This must be achieved while minimizing defects such as inhomogeneities, unmelted batch materials, forming defects, devitrification, or gaseous inclusions. Manufacturing must also be achievable in a cost-effective manner to ensure profitability. As indicated in Fig. 2, some important manufacturing-related properties include viscosity, liquidus temperature, forming temperature, refractory compatibility, and batch cost.

## 3. Model-driven glass design

Given a desired set of product- and manufacturing-related attributes that must be achieved, how can one obtain an optimized composition satisfying all of these requirements? Historically, researchers employed the so-called "cook and look" approach of glass design. Based on many years of knowledge and intuition and the available data in literature and lab notebooks, researchers would take an educated guess at an initial glass composition. This composition would be prepared in a crucible melt, and the resulting glass would be characterized to measure the relevant properties of interest. Comparing the actual measured properties with the desired properties, the researcher would then conduct additional crucible melts until the target properties are achieved. While historically successful for a number of glass products, the "cook and look" approach is inefficient and expensive, and it cannot ensure that a truly optimized glass composition is obtained.

An alternative approach is the model-driven design of new glass compositions, in which quantitatively accurate models are developed for each relevant property [13]. Each model is a function of a common set of variables, e.g., the concentration of each chemical component in the glass. The models are then incorporated into a mathematical optimization routine, as indicated in Fig. 3. For the optimization to proceed, a target function (or property) must be specified. The target function is then either maximized or minimized (as appropriate) by adjusting the composition of the glass, subject to a set of constraints on other relevant properties that are needed to meet the remaining product- and manufacturing-related attribute requirements.

This constrained optimization process can be conducted using deterministic techniques such as steepest descent or the Newton-Raphson method [19], or it can proceed following a stochastic algorithm such as simulated annealing [20]. Stochastic

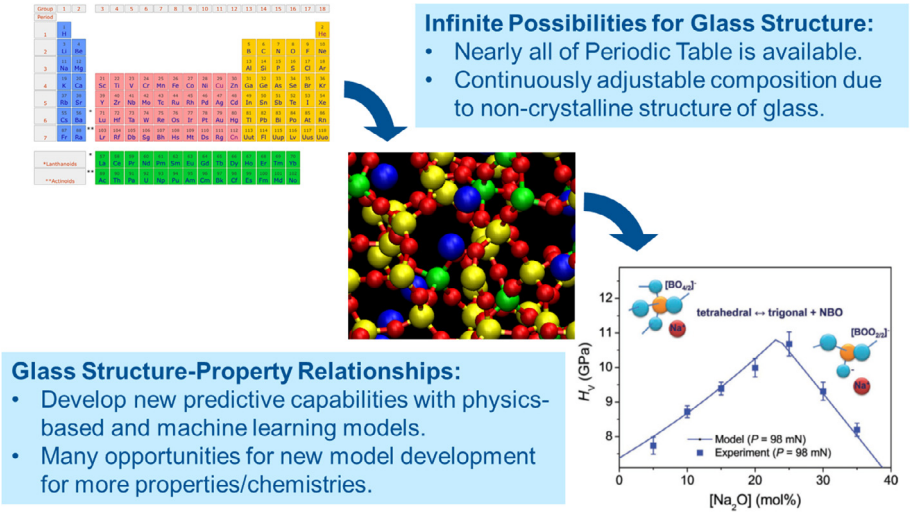


**Fig. 1.** Given the essentially infinite number of possible glass structures available, the task of designing new glass compositions can be potentially daunting. A combination of physics-based and empirical modeling approaches can be used to help design new glasses with targeted property values. For example, topological constraint theory can be used to give quantitatively accurate predictions of glass hardness (right plot) based on structures determined either experimentally or through atomic level simulations (middle plot).

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