Acta Biomaterialia 8 (2012) 2324–2330

Contents lists available at SciVerse ScienceDirect

Acta Biomaterialia

journal homepage: www.elsevier.com/locate/actabiomat

Regression model for predicting selected thermal properties of next-generation bioactive glasses

S.M. Breed, M.M. Hall *

Alfred University, Inamori School of Engineering, 2 Pine Street, Alfred, NY 14802, USA

ARTICLE INFO

Article history:
Received 28 August 2011
Received in revised form 10 December 2011
Accepted 7 February 2012
Available online 13 February 2012

Keywords:
Bioactive glass
Thermal expansion coefficient
Glass transition temperature
Regression analysis
Thermal properties

ABSTRACT

The compositional palette traditionally used to develop bioactive glasses has grown in recent times to include therapeutic inorganic species such as zinc and strontium. Historical regression models used for predicting the properties of bioactive glasses as a function of composition have not evolved to consider this expanded compositional space. In this work, nonlinear regression analysis was applied to historical data to construct predictive models for the glass transition temperature and the coefficient of thermal expansion of next-generation bioactive glasses. The new regression models also provide some degree of improvement over existing models in predicting the properties of traditional bioactive glasses.

1. Introduction

Bioactive glasses are generally recognized as materials for hard tissue replacement and repair [1]. The functionality of bioactive glasses has more recently been extended into other applications, primarily by expanding upon the traditional compositional palette consisting of oxides such as Na_2O, K_2O, MgO, CaO, B_2O_3, P_2O_5, and SiO_2. The incorporation of new functionality is largely motivated by the recognition that dissolution products from bioactive glasses can provide therapeutic benefits [2]. For example, zinc-doped and strontium-doped bioactive glasses are being actively investigated. Zinc is a well-known promoter of bone formation [3–7]. Zinc-releasing glasses have also shown anti-inflammatory [8,9] and anti-bacterial properties [10–12]. Strontium-releasing glasses have more recently been developed owing to their ability to stimulate osteoblasts while inhibiting osteoclasts [13,14], properties that can be leveraged in osteoporotic patients [15–17].

Bioactive glasses are employed in a variety of forms, including particulate, fiber, and coatings. Bioactive glass coatings can be applied to implant materials having beneficial mechanical properties but limited ability to integrate with hard tissue, including most metallic alloys and structural ceramics [18–21]. In addition to the baseline bioactivity of the glass, a number of additional functional requirements must be considered when designing bioactive glasses for coating applications – e.g. compatible thermal expansion behavior, compatible processing temperatures, stability against devitrification, and good wetting and bonding characteristics.

Multi-component glasses are typically required when attempting to satisfy multiple property requirements. The formulation of an optimal multi-component glass that simultaneously satisfies multiple property requirements cannot easily be accomplished using a rational design approach rooted in basic knowledge of glass structure. For example, one might reasonably choose to increase the coefficient of thermal expansion (CTE) of a silicate-based glass by increasing the network modifier content [22]. However, in order to meet a specific CTE target, significant questions remain about the choice of modifier(s) and the exact amount to be added. In practice, the optimization of multi-component glasses having precisely specified properties often requires a statistics-based approach [23], the product of which is regression models for predicting the compositional dependence of glass properties such as CTE and the glass transition temperature (T_g).

Prior groups have recognized the utility of developing regression models for predicting the compositional dependence of various properties of bioactive glasses, including: viscosity–temperature behavior (including specific points such as T_g and dilatometric softening temperature), CTE, crystallization behavior, in vitro bioactivity, and in vivo bioactivity [24–34]. The regression model for T_g can simply be applied to the determination of annealing schedules, particularly when preparing new compositions for which experimentally measured T_g data are not immediately available. A combination of models for CTE and T_g can also be used in developing bioactive glass formulations for coating applications.

* Corresponding author. Tel.: +1 607 871 3143; fax: +1 607 871 2354.
E-mail address: hallmm@alfred.edu (M.M. Hall).

1742-7061/$ - see front matter © 2012 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
doi:10.1016/j.actbio.2012.02.009