Practical IR extinction coefficients of water in soda lime aluminosilicate glasses determined by nuclear reaction analysis

Toshio Suzuki a,⁎, Junko Konishi a, Kiyoshi Yamamoto b, Shohei Ogura b, Katsuyuki Fukutani b

a Research Center ASAM Glass Co., Ltd., 1159 Hazawa-cho, Kanagawa-ku, Yokohama-shi, Kanagawa 222-8755 Japan
b Institute of Industrial Science, The University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8505 Japan

Article history:
Received 4 September 2013
Received in revised form 13 October 2013
Available online 5 November 2013

Abstract

Infrared absorption spectroscopy (IR) is widely used to determine the water content in glasses, whereas determination of the practical extinction coefficient is necessary to deduce the absolute water concentration of glasses on the basis of Beer-Lambert law. On the basis of the nuclear reaction analysis (NRA) data, the IR practical extinction coefficient of water was successfully determined for the glasses with different levels of Al contents. Whereas the two-band method is well known to determine the water concentration in alkali lime silica glasses, we show that the single-band procedure with a practical absorption coefficient is suitable for the determination of the water concentration in soda lime aluminosilicate glasses containing substantial amounts of Al content. A good correlation is confirmed between the non bridging oxygen/terahedral cations (NBO/T) ratio and the practical extinction coefficient of water in soda lime aluminosilicate glasses with identical network-modifying cations.

© 2013 Elsevier B.V. All rights reserved.

1. Introduction

The water content in glasses, equivalent to the SiOH or silanol group, significantly influences the glass properties such as viscosity, strength, and optical property. The water concentration in glasses is often estimated by infrared absorption spectroscopy (IR) following the Beer-Lambert law expressed by Eq. (1) [1–3].

\[ \text{CH}_2\text{O} = A / \left( \varepsilon_{\text{practical}} \cdot d \right) \]

(1)

where \( \text{CH}_2\text{O} \) (mol·l⁻¹) is the water concentration, \( A \) is the absorbance, \( d \) (cm) is the glass thickness, and \( \varepsilon_{\text{practical}} \) (mol⁻¹·cm⁻¹) is the practical extinction coefficient. Whereas the IR method is quick, inexpensive and convenient to derive the water content in glasses, the absolute water concentration cannot be obtained only with the IR method. Determination of the IR practical extinction coefficient is necessary to deduce the absolute water concentration.

In previous studies, the practical extinction coefficient was determined by vapor pressure, gravimetry and degassing methods [4–6] for alkali lime silica and/or silica glasses. These analytical methods can obtain the water concentration by measuring the water vapor quantity or the weight loss of glass samples due to heat treatment above the glass transition temperature. Although they are powerful to determine the water concentration in glasses, much trial and high degree of skill are necessary to obtain reliable data because dehydroxylation of silanol groups leads to deformation of the glass sheet and bubble generation, which makes IR measurements troublesome.

The IR spectrum of alkali lime silica glasses reveals two absorption bands at 3550 and 2800 cm⁻¹, which are attributed to the very weakly associated “free” OH groups and strongly associated OH groups in silanol forms, respectively. To accurately correlate the extinction with the water concentration in alkali lime silica glasses, the two-band method was proposed by Scholze [4]. According to this method, the total water concentration, \( \text{CH}_2\text{O} \), of glasses is calculated by Eq. (2) with the extinction coefficients \( \varepsilon_{3550} \) and \( \varepsilon_{2800} \) of the silanol bands at 3550 and 2800 cm⁻¹, respectively.

\[ \text{CH}_2\text{O} = \frac{1}{d} \left( \frac{A_{3550} - A_{2800}}{\varepsilon_{3550}} + \frac{4}{3} \frac{A_{2800} - A_{1500}}{\varepsilon_{2800}} \right) \]

(2)

Here, \( A_{1500}, A_{2800} \) and \( A_{3550} \) denote the absorbance at wavenumbers of 3550, 4000, and 2800 cm⁻¹, and \( d \) is the glass thickness. The extinction coefficients are given at \( \varepsilon_{2800} = 150 \) and \( \varepsilon_{3550} = 70 \) (mol⁻¹·cm⁻¹), which were obtained with the water concentration determined by the vacuum-degassing process [4,6].

Harder et al. reported the water concentration in soda lime silica (SLS), potassium lime silica (KLS) and cesium lime silica (CLS) glasses by using nuclear reaction analysis (NRA) with the resonant nuclear reaction of \( ^{1}H(p, \gamma) ^{2}H \) [7,8], which allows for measurements of the absolute hydrogen concentration. It was confirmed that the water concentration obtained by the IR two-band method gave values 8% larger than that of determined with NRA when no band separation procedure was applied.

⁎ Corresponding author. Tel.: +81 45 375 7332; fax: +81 45 375 8802.
E-mail address: toshio-suzuki@asam.co.jp (T. Suzuki).
0022-3093/© 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.jnoncrysol.2013.10.011

- 66 -