UNIVERSITI TEKNOLOGI MARA

EFFECTS ON VIBRATIONAL ENERGY, ELECTRONIC AND OPTICAL PROPERTIES OF SiO_2 GLASS INCORPORATED WITH ALUMINA

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May 2018

ABSTRACT

SiO_2 glass is one of the most used material in optical applications since it possess excellent properties such as exhibits ultra-low-optical loss of 0.2 dB/km at wavelength of 1.55 μm and highly transparent across a broad range of wavelengths. Doping of RE ion into SiO_2 glass is necessary as an optical activator in SiO_2-based devices. However, SiO_2 glass suffers from high phonon energy, of about 1100 cm^{-1} that affects the emission of RE ion. Since SiO_2 glass has high phonon energy and the RE ion itself has a non-radiative emission, thus photon emission has to compete with this vast amount of phonon. From the relationship of non-radiative decay rate, incorporating lower phonon energy material into SiO_2 glass would change its phonon energy. Al_2O_3 is one of the favourable glass intermediate to be incorporated into SiO_2 glass since it has lower phonon energy than SiO_2 glass that is 780 cm^{-1}. However, the incorporation of Al_2O_3 in SiO_2 glass will lead to phase separation if the amount of Al_2O_3 exceeds certain amount of ratio. Experimental works show variation in the molar ratio of SiO_2-Al_2O_3 composition from 0 to 90% which are due to the different experimental techniques and initial treatments to the sample. Therefore, it is necessary to find the theoretical limit of SiO_2-Al_2O_3 since there is no available work on finding the optimum ratio of SiO_2-Al_2O_3 by theoretical approach. In this present work, small sample of SiO_2 glass was successfully been generated using Rietveld refinement technique and calculated using density functional theory (DFT) framework. A thorough analysis on the properties of SiO_2 glass structure are validated with previous works and serve as a reference to analyse the effect of Al_2O_3 on the vibrational, electronic and optical properties of SiO_2 glass besides to determine the optimal composition of SiO_2-Al_2O_3 system. The composition of Al_2O_3 has been limited to a desired amount so as not to perturb other properties of SiO_2. The Infrared (IR) and Raman spectra for SiO_2-Al_2O_3 systems were simulated at different molar ratio using Molecular Mechanics framework. It has been found that phonon energy of SiO_2 glass has been reduced as the intensity of ~1091 cm^{-1} band is reduced about 50 % with the proportion of 20 mol % Al_2O_3 in SiO_2 host. The decreasing in intensity of ~1091 cm^{-1} band demonstrates the formation of Al-O-Si linkages in the structure. However, upon further addition of 50 mol % of Al_2O_3, the development of Al-O-Al bond can be observed which indicates the occurrence of phase separation phenomena. The structure also tends to exhibit similar electronic and optical properties with that pure SiO_2 system.

ACKNOWLEDGEMENT

Firstly, I wish to thank God for giving me the opportunity to embark on my Msc and for completing this long and challenging journey successfully. My gratitude and thanks go to my supervisor Prof Dr Mohd Kamil bin Abd Rahman for his patience, motivation, and immense knowledge. The door to his office was always open whenever I ran into a trouble spot or had a question about my research or writing.

My appreciation goes to my first co-supervisor, Dr Mohamad Fariz bin Mohamad Taib who provided the facilities, encouragement and assistance during my MSc journey. Special thanks to my second co-supervisor, Dr Abdel Baset, who provided the insight and expertise that greatly, assisted this research.

I must express my very profound gratitude to my family and to my team mate, Siti Nabilah binti Mohd Halim for providing me with unfailing support and continuous encouragement throughout my years of study and through the process of researching and writing this thesis. I would also like to thank all my friends who always delighted to offer me their helps and moral supports during the hardship of this study.This accomplishment would not have been possible without them.

I am highly indebted to distinguished members of the panel for the approval of my work. Many thanks to the MOHE for funded my study. Last but not least, I would like to thanks all people who have willingly helped me out with their abilities and support in completing my endeavour.

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CHAPTER ONE
INTRODUCTION

1.1 RESEARCH BACKGROUND

Solid material is categorized according to the arrangement of atoms in the structure. Solid can be classified into two types, which are crystalline and non-crystalline materials. Crystalline solid is referring to the symmetrical and regular pattern of atomic arrangement. Non-crystalline is generally known as amorphous solid material. Atoms in non-crystalline solid are in irregular manner (disordered), without short or long-range order atomic arrangement. The physical structure of both solid materials are compared in the Figure 1.1.

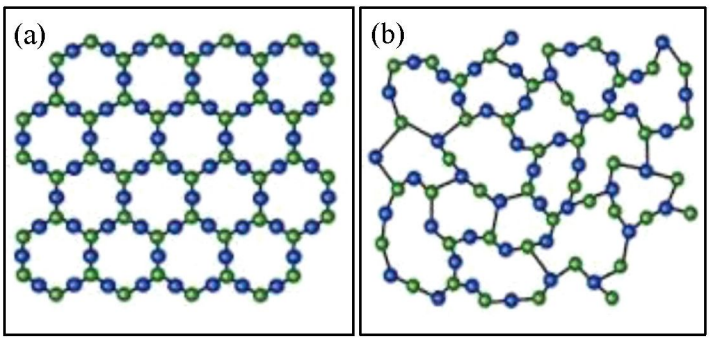

Figure 1.1: Atomic arrangement of (a) Crystalline structure & (b) Amorphous structure (glass)

Glass is regarded as a non-crystalline material due to the lack of symmetry in its structure (Debenedetti & Stillinger, 2001). Both crystalline and glass form share a similar characteristic of the three-dimensional network structure. The structural units of glass are been randomly linked together to form a non-periodic arrangement of the molecules (Dove, Han, Wallace, & De Yoreo, 2008).

Glass has been an interest to everybody in this world since around 5000BC (Kulshreshtha & Vasile, 2002). The earliest glass making was begun in Egypt and Eastern Mesopotamia (Davison & Newton, 2008). The first glassmakers were motivated to create decorative objects, possibly to simulate gems and semiprecious stones, using sintered bodies of silica and desert soda with appropriate colorants, such as copper, manganese, and iron salts (Kurkjian & Prindle, 1998). There was no evidence confirming the interest in transparency at this time.