

# Structure and Elasticity of Silicate Glasses and Supercooled melts

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## Abstract

The effects of composition, temperature, and cationic size on the structure and elastic properties of glasses and supercooled melt have been studied using both Brillouin and Raman scattering techniques. Relative to Na<sub>2</sub>O-SiO<sub>2</sub> glasses, the maximum abundance for Q<sup>3</sup> and Q<sup>2</sup> in the present glasses shows a lag of 0.5 NBO/Si units. This phenomenon has been correlated to the possible change in average coordination number of Na<sup>+</sup> ions due to the presence of Mg<sup>2+</sup>. Taking the lag of 0.5 NBO/Si into account, all the three Q<sup>n</sup> ↔ Q<sup>n+1</sup> + Q<sup>n-1</sup> (n=1, 2, 3) equilibria in Na<sub>2</sub>O-SiO<sub>2</sub> glasses were shifted to the right due to the addition of MgO. The acoustic data have revealed that both shear and Young's moduli of the present glasses decrease with increasing in NBO/Si, while the reverse variation was observed in bulk modulus. By considering the factors determining the elastic properties of a glass and the relative changes in the amounts of Q species and shear modulus, the effect of Q species resistant to shear deformation of a silicate glass has the order: Q<sup>4</sup> > Q<sup>3</sup> > Q<sup>2</sup> > Q<sup>1</sup> and Q<sup>0</sup>. Except for the abnormally low moduli in Mg-bearing glass, that the elastic moduli of glasses decrease with increasing in size of M<sup>2+</sup> cation can be attributed to the competition between increase of density and lowering in field strength of alkaline earth cations. The compiled data of alkali silicate glasses showed that each kind of glass displays different M<sub>2</sub>O concentrations for getting minimum bulk modulus due to difference in field strength of cations, depolymerization of silicate network, and coordination number of cations. The specific M<sub>2</sub>O concentrations for such minima increase with increasing cation size. Different composition dependences of elastic moduli for the glasses having same constituents can be ascribed to different mechanisms for compression and shear deformation.

For basaltic glasses, the elastic moduli decrease with increasing SiO<sub>2</sub> concentration. The shear moduli displayed the least dependence on SiO<sub>2</sub> content. The bulk moduli of the basaltic glasses strongly depend on the sum of the Q<sup>3</sup> and Q<sup>4</sup> anionic units. Among the modifiers, iron cations showed the strongest effect on the elastic properties of the rhyolitic glasses. For the elastic moduli of rhyolitic glasses, the major effect of alkaline earth cations is on shear modulus; however, both iron and alkali cations showed stronger effects on bulk modulus and similar relative contribution between bulk and shear moduli. The dependences of elastic moduli on bulk NBO/T observed in both types of aluminosilicate glasses suggest that the elastic modulus of a glass depends on the concentration of effective modifying cations rather than the apparent concentration of all non-network-forming cations. Upon heating, the elastic moduli of an iron-bearing rhyolitic glass showed weak temperature dependences below its glass transition temperature (T<sub>g</sub>) and fasterly drop above T<sub>g</sub>. This glass gradually darkened above 850 °C (~T<sub>g</sub>) due to crystallization of magnetite (Fe<sub>3</sub>O<sub>4</sub>). Unlike those reported for the iron-free samples, crystallization of magnetite in this supercooled melt at high temperatures (> 1000 °C) caused an apparent increase in elastic moduli. This result indicates that iron oxides cannot be neglected for simulating the elasticity of volcanic glasses at high T. Furthermore, a test to the ideal mixing model has revealed that an accurate prediction in Young's modulus and density using the Makishima-Mackenzie relationship and partial molar volumes is not successful for both the ternary and multicomponent aluminosilicate glasses studied.