American Mineralogist, Volume 93, pages 946–949, 2008

LETTER

Evidence for anomalously large degree of polymerization in Mg_2SiO_4 glass and melt

SABYASACHI SEN[1,*] AND JEAN TANGEMAN[2]

[1]Department of Chemical Engineering and Materials Science, University of California at Davis, Davis, California 95616, U.S.A.
[2]3M Corporate Research Laboratory, St. Paul, Minnesota 55144, U.S.A.

ABSTRACT

Ab-initio molecular dynamics simulation of forsterite (Mg_2SiO_4) melt at 2273 K shows the presence of nearly 40% of the Si atoms as $(Si_2O_7)^{6-}$ dimers. This result is directly corroborated by the ^{29}Si nuclear magnetic resonance spectrum of bulk Mg_2SiO_4 glass, prepared by container-less levitation techniques. The presence of a large excess of bridging O atoms associated with the $(Si_2O_7)^{6-}$ dimers in forsterite glass and melt is in sharp contrast with their complete absence in crystalline forsterite. Such structural differences between the crystal and the melt can have important implications in understanding the dynamics of crystallization and segregation in a primordial magma ocean and the continuing chemical differentiation of the Earth.

Keywords: Ab initio molecular dynamics, forsterite, melt, glass, simulation, NMR, structure