

Structural simulation on silica crystals and glasses

TAKADA¹

¹Research Center, Asahi Glass Co., 1150 Hazawa-cho, Yokohama, 221-8755, Japan (akira-takada@agc.com)

Molecular dynamics simulation has been used to investigate the similarity and dissimilarity in dynamical structural changes between silica crystals and glasses. Many simulation studies have been performed for quartz, cristobalite and silica glasses [1-3], however, there is scarcely any simulation studies on tridymite. The structural building block is the same between in tridymite and cristobalite, nevertheless, structural changes due to the thermal effects is more complex in tridymite than in cristobalite. Such complexity hinders the theoretical study. First, the structural changes of tridymite phase due to thermal effects are investigated by using molecular dynamics simulation. Next, the calculated complex structural changes are compared with those of the other structures such as cristobalite and glasses. Finally, we discuss the similarities and dissimilarities in dynamical structural changes in terms of microscopic structure.

[1] A. Takada, P. Richet, C.R.A. Catlow, G.D. Price (2004) *J. Non-Cryst. Solids* 345&346, 224. [2] A. Takada, P. Richet, C.R.A. Catlow, G.D. Price (2007) *J. Eur. J. Glass Sci. Technol. B* 48, 182. [3] A. Takada, P. Richet, C.R.A. Catlow, G.D. Price (2008) *J. Non-Cryst. Solids* 354, 181.

Ontogenetic stable isotope records of modern planktic foraminifers from Sagami Bay, Japan

H. TAKAGI^{1*}, K. MORIYA^{1,2}, T. ISHIMURA^{3,4}, A. SUZUKI⁴
H. KAWAHATA⁵ AND H. HIRANO¹

¹Waseda University, Tokyo 169-8050, Japan

(*correspondence: harurah-t@fuji.waseda.jp)

²Kanazawa University, Kanazawa 920-1192, Japan

³Ibaraki National College of Tech., Ibaraki 312-8508, Japan

⁴Geological Survey of Japan, AIST, Ibaraki 305-8567, Japan

⁵AORI, The University of Tokyo, Chiba 277-8564, Japan

Stable oxygen ($\delta^{18}\text{O}$) and carbon ($\delta^{13}\text{C}$) isotopes recorded in planktic foraminiferal tests are widely used as proxies for paleoceanography and species ecology. Of such isotopic investigations, ontogenetic isotopic profiles are thought to record foraminiferal ecological information such as depth habitat or symbiotic relationship. Though size-related isotopic series, achieved by analyses of a series of sieved fractions, seem to reflect ontogenetic profiles of species, isotopic profiles through "individual ontogeny" have rarely been examined. In this study, we report ontogenetic isotopic information of individual specimens, together with *in situ* water column oceanographic information ($\delta^{18}\text{O}_{\text{sw}}$, $\delta^{13}\text{C}_{\text{DIC}}$, temperature, salinity, nutrient, and chlorophyll-a).

We examined ontogenetic stable isotopic profiles of planktic foraminifers by performing chamber-by-chamber analyses within a single individual. Each chamber is dissected from an individual and analyzed by specially designed continuous-flow mass spectrometry system [1]. Instead of size-related analyses, this method enables us to reveal individual ontogenetic information free from mixing of seasonal variability. Four modern species, obtained by vertical towing at Sagami Bay, Japan, were analyzed; *Globigerinoides sacculifer*, *Globigerinoides conglobatus*, *Neoglobobulimina dutertrei*, and *Globobulimina inflata*.

The ontogenetic $\delta^{18}\text{O}$ profiles showed overall increase for all species, suggesting the ontogenetic deeper migration commonly found in modern species. While $\delta^{13}\text{C}$ showed steep increase especially in a juvenile stage for all species, the increase continued to the last chambers only in symbiont-bearing globigerinoidid species. $\delta^{13}\text{C}$ of asymbiotic species becomes decrease after the rapid increase in the juvenile stage. Comparing these records to water column chemical and physical data, regardless of their adult habitat depths, all foraminifers analyzed start their calcification, hence their ontogeny, near the thermocline, which corresponds to chlorophyll maxima and nutrient-depleted depth.

[1] Ishimura *et al.* (2004), *RCM*, 22, 1925-1932.