

Local Structure Analysis of Non-Crystalline Materials based on PDFs

Akito Sasaki, Akihiro Himeda, Norihiro Muroyama, Yuji Shiramata, Keisuke Saito

Rigaku Corporation

a-sasaki@rigaku.co.jp

PDF is often used for the analysis of, in particular, non-crystalline materials which do not have 3-dimensional periodic structures, since PDF provides you with an important information to analyze the local structures of materials. The scattering patterns till high Q-ranges are required to obtain high r -resolution PDF, therefore, the first choice to measure such a high-Q data used to be a synchrotron facility where short wavelengths are available. Today, it is getting easier to make measurements till relatively high Q-ranges using the Mo or Ag wavelengths even with in-house X-ray diffractometers. Thus, the analysis based on PDF is getting more popular.

Figure 1 shows the analysis result of the network structure of non-crystalline soda glass using an RMC method based on PDF, which was calculated from a diffraction pattern of the soda glass with the Mo wavelengths. It is well-known that silicon atoms and oxygen atoms in quartz form 8- or 12-membered rings, on the other hand, it is indicated that some of the rings are broken due to the existence of sodium atoms. It is quite interesting that the obtained structure is similar to the calculated one. We will do further analysis by, for example, increasing the number of atoms, and will make a presentation on the local structure analysis of non-crystalline materials based on PDF. In addition, we will introduce in-house X-ray diffractometers and their optics on which we have been focusing to obtain good PDFs, that is, to obtain good scattering patterns for such this kind of analysis,

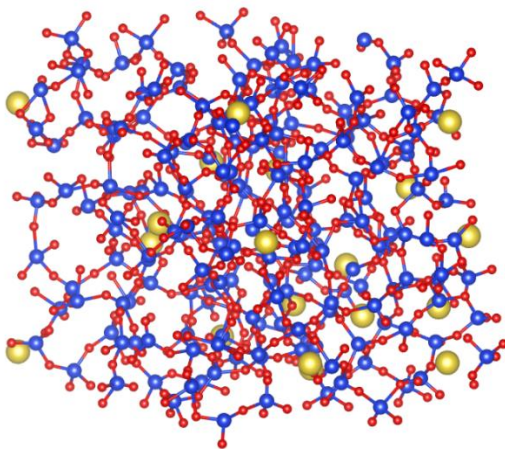


Figure 1. Network structure of non-crystalline soda glass

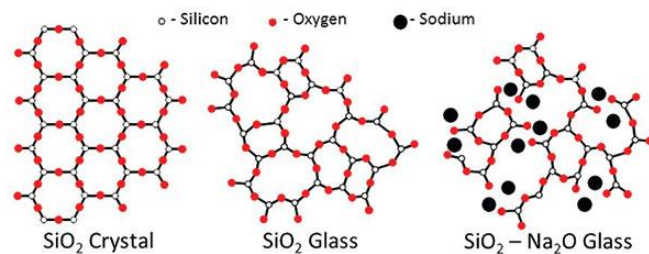


Figure 2. Predicted structures