Compression behaviour and pressure-induced strain of icosahedral Zn-Mg-Y quasicrystal

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Abstract. The compression behaviour and pressure-induced disorder of an icosahedral Zn₅₅Mg₃₅Y₁₀ quasicrystal has been investigated by means of an in-situ angle-dispersive X-ray powder diffraction method using synchrotron radiations. The icosahedral structure was found to be essentially stable under high pressures up to 70 GPa and at 1 bar after recovered from 70 GPa. However, it should be noted that all peaks of the X-ray diffraction after recovered were broad even at 1bar. This indicates that the recovered sample contains a lot of pressure-induced strains even though it was an icosahedral quasicrystal. It was found that there was a linear relation between Q// (physical momentum) and HWHM (Half Width at Half Maximum) of the X-ray diffraction peaks of the sample recovered from 70 GPa. On the other hand, there was no correlation between Q⊥ (phason momentum) and HWHM. In addition, there was no linear relation between (Q⊥/Q//)² and (HWHM/Q//)². These analyses indicate that the pressure-induced strains in the extremely strained Zn-Mg-Y quasicrystal recovered from 70 GPa are explained by neither of the icosahedral glass nor the frozen-in phason strain models, and explained well by the simple lattice (phonon) strain.

1. Introduction
Since the discovery of quasicrystals a lot of researches on the stability against temperature have been reported. On the other hand, only limited researches on the stability against pressure have been reported. A pressure induced phase transition from quasicrystal to amorphous on icosahedral (i-) Al-Li-Cu quasicrystal at 13 GPa at room temperature was reported by Akahama et al. [1]. However, other various kinds of quasicrystals were reported to be stable at high pressures [2-14], such as i-Al-Mn, i-Al-Cu-Fe, i-Al-Cu-V, i-Al-Cu-Cr, i-Al-Cu-Mn, i-Al-Pd-Mn, i-Al-Pd-Re, i-Al-Ru-Cu, i-Ti-Zr-Ni, i-Cd-Ca etc. We have also reported the high stability of decagonal Al₇₅Ni₂₅Co₅, i-Al₇₂Pd₁₈.₅Mn₉.₅ and i-Zn₅₅Mg₃₅Y₁₀ under high pressures up to about 70 GPa [15-17].

Although they keep the icosahedral structure essentially at high pressures and after recovered from high pressure, all peaks of the X-ray diffraction were broad even at 1bar. This indicated that they contained a lot of pressure-induced strains even though they were icosahedral quasicrystals. This indicates that the recovered sample contains a lot of pressure-induced disorders even though it was an

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icosahedral quasicrystal. Two types of disorders: icosahedral glass and frozen-in phason strain, in non-compressed quasicrystals of the Al-Mn system were suggested by Horn et al. [18]. They analyzed momentum (physical momentum (real scattering vector): Q∥, phason momentum: Q⊥) dependence of linewidth of X-ray diffraction data. The frozen-in phason strain was reported on other quasicrystals such as \( i\text{-Al}_{65}\text{Cu}_{20}\text{Fe}_{15} \) [19] and \( i\text{-Al}_{70}\text{Pd}_{20}\text{Mn}_{10} \) [20]. High pressure measurements over 50 GPa are usually performed under non-hydrostatic conditions. Thus, it is easily expected that quasicrystals recovered from high pressures include a lot of disorders in an atomic level. In this paper disorders in \( i\text{-Zn}_{55}\text{Mg}_{35}\text{Y}_{10} \) recovered from 70 GPa have been described on the basis of analyses of the linewidth of the diffraction peaks in the X-ray powder diffraction pattern.

2. Experimental procedure

The \( i\text{-Zn}_{55}\text{Mg}_{35}\text{Y}_{10} \) sample was a powder of a polygrained quasicrystal. Alloying was performed in a pyrolytic boron-nitride crucible in an argon atmosphere using a high-frequency furnace. The sample was characterized by TEM and back-Laue X-ray diffraction. They revealed high quasicrystallinity and good homogeneity. The details of the grown procedure and characterization results were reported elsewhere [21]. The powder sample used for the X-ray experiments were prepared by grinding the prepared quasicrystals gently in an agate mortar. The phase identification after grinding was made by the X-ray diffraction and electron diffraction, showing a single phase of quasicrystal and high quasicrystallinity.

High pressure X-ray diffraction experiments were performed using a lever and spring-type diamond anvil (culet size: 350 \( \mu \text{m} \) in diameter) apparatus [22] and stainless steel gasket (gasket hole: about 150 \( \mu \text{m} \) in diameter). No pressure medium was used. The pressure was measured using the ruby fluorescence technique. Some ruby chips were arranged on the surface of the sample. A ruby chip placed near the center of the sample chamber was used for pressure measurements. High resolution angle dispersive X-ray diffraction experiments were carried out using synchrotron radiation at the Photon Factory, National Laboratory for High Energy Physics (KEK) in Tsukuba. A monochromatized X-ray of wavelength 0.4817 Å was collimated to a thin beam (30 \( \mu \text{m} \) x 30 \( \mu \text{m} \)) to get the diffraction pattern from the limited narrow region of the sample around the ruby chip pressure marker. The diffracted X-ray was detected by an imaging plate (IP). In order to obtain high resolution and accuracy, the IP detector was placed about 320 mm apart from the sample. X-ray intensities recorded in each pixel of the IP were measured by a laser-scanning reader and converted into two-dimensional digital intensity data. These data were then integrated along a polar axis which coincided with the Debye rings observed on the IP, and the powder diffraction intensities were obtained as a function of 2θ angle. An exposure time was about 1 hour. The details of the data analysis was described elsewhere [23]. The X-ray diffractions were taken at pressures below about 70 GPa.

3. Results and discussion

Figure 1 shows some of the pressure dependence of the measured X-ray diffraction patterns. The diffraction pattern of the recovered sample is also shown in the figure. All measured patterns were found to intrinsically correspond to the icosahedral-type quasicrystal. This indicates that this quasicrystal is stable below 70 GPa. The zero-pressure bulk modulus, \( B_0 \) were calculated by fitting the pressure dependence of \( (dV/d\rho)_{\text{ave}} \) instead of \( V/V_0 \), using the Birch-Murnaghan equation. The calculated \( B_0 \) and its pressure derivative are 73 ± 1 GPa and 3.6 ± 0.1, respectively.

Although the diffraction patterns of the recovered sample correspond to the icosahedral quasicrystal structure essentially, all peaks of the X-ray diffraction are broad even at 1 bar. This indicates that the recovered sample contains a lot of disorders even though it is an icosahedral quasicrystal. As mentioned in the introduction, Horn et al. discussed disorders in quasicrystals on the basis of plots for two possible types of disorder in Mn-Al quasicrystals [18]. One type is an icosahedral glass. In this case, HWHM (Half Width at Half Maximum) is proportional to \( Q_\perp^{2k} \) (k:constant). Figure 2 shows the \( Q_\perp \) dependence of HWHM for the recovered sample. Since it is
difficult to find any correlations between $Q_\perp$ and HWHM in Figure 2, the pressure-induced disorders of the recovered $i$-Zn$_{55}$Mg$_{35}$Y$_{10}$ are not of the icosahedral glass. The other one is a frozen-in phason strain. In this case, there is a linear relation between $(Q_\perp/Q_\parallel)^2$ and $(HWHM/Q_\parallel)^2$. Such a linear relation was actually reported for the non-compressed $i$-Al$_{65}$Cu$_{20}$Fe$_{15}$ [19] and non-compressed $i$-Al$_{70}$Pd$_{20}$Mn$_{10}$ [20]. Figure 3 shows the relation between these parameters for the recovered sample in this study. Since the data points cluster at low $(Q_\perp/Q_\parallel)^2$, a log-log plots are also shown in the inset of the figure. It is found that there is no linear relation between these two parameters. This also means that pressure-induced disorders in the recovered $i$-Zn$_{55}$Mg$_{35}$Y$_{10}$ were not of the frozen-in phason strain. Therefore, it is concluded that the disorders in the $i$-Zn$_{55}$Mg$_{35}$Y$_{10}$ recovered from 70 GPa are neither icosahedral glass nor frozen-in phason strain.

Although there is no correlation between $Q_\perp$ and HWHM, it should be noted that there is a clear linear relation between $Q_\parallel$ and HWHM, as shown in Figure 4, i.e. $HWHM = \alpha Q_\parallel + \beta$ where $\alpha$ and $\beta$ are 0.0058(4) and 0.0055(14), respectively. This linear relation indicates that the peak broadening of the recovered $i$-Zn$_{55}$Mg$_{35}$Y$_{10}$ is accounted for by the simple lattice strain. The same linear relation was reported for the non-compressed $i$-Al$_{65}$Cu$_{20}$Ru$_{15}$ [24], and the parameters $\alpha$ and $\beta$ were 0.000475(5) and 0.00049(1), respectively. It should be noted that the values in our study are almost 12 times larger than those of the $i$-Al$_{65}$Cu$_{20}$Ru$_{15}$. This means that the structure of the recovered $i$-Zn$_{55}$Mg$_{35}$Y$_{10}$ is
extremely strained even though it still keeps the icosahedral quasicrystal structure. It is interesting that the phason strains are not observed even in such an extremely strained quasicrystal.

4. Conclusion
The compression behaviour of an icosahedral Zn-Mg-Y quasicrystal has been investigated by means of an in-situ angle-dispersive X-ray powder diffraction method using synchrotron radiations. Powdered samples were compressed directly using diamond anvil up to 70 GPa. The icosahedral structure was found to be essentially stable under high pressures up to 70 GPa and at 1 bar after recovered from 70 GPa. All broad X-ray diffraction peaks after recovered indicated that the recovered sample contained a lot of pressure-induced strains. It was found that there was a clear linear relation between Qₚ and HWHM of the X-ray diffraction peaks of the recovered sample, while there was no correlation between Q₀ and HWHM. In addition, there was no linear relation between (Q₀/Qₚ)² and (HWHM/Q₀)². These analyses indicate that the pressure-induced strains in the extremely strained Zn-Mg-Y quasicrystal recovered from 70 GPa are explained by neither of the icosahedral glass nor the frozen-in phason strain models, and explained well by the simple lattice (phonon) strain.

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References
[1] Akahama Y, Mori Y, Kobayashi M, Kawamura H, Kimura K and Takeuchi S 1989 J. Phys. Soc. Jpn. 58 2231
[2] Sadoc A, Itie J P, Polian A and Lefebvre S 1996 Phil. Mag. A 74 629
[3] Sato-Sorensen Y and Sorensen L B 1989 Phys. Rev. B39 2654
[4] Kang S S and Dubois J M 1992 Europhys. Lett. 18 45
[5] Sadoc A, Itie J P, Polian A, Lefebvre S, Bessiere M and Calvayrac Y 1994 Phil. Mag. B 70 855
[6] Lefebvre S, Bessiere M, Calvayrac Y, Itie J P, Polian A and Sadoc A 1995 Phil. Mag. B 72 101
[7] Ponkraz U, Nicula R, Jianu A and Burkel E 2001 J. Phys. : Cond. Matt. 13 549
[8] Amazit Y, Perrin B, Fischer M, Itie J P and Polian A 1997 Phil. Mag. A 75 1677
[9] Decremps F, Gauthier M and Richebourg F 2006 Phys Rev. Lett. 96 105501
[10] Sadoc A, Itie J P, Polian A, Berger C and Poon S J 1998 Phil. Mag. A 77 115
[11] Sadoc A, Itie J P and Polian A 2000 Phil. Mag. A 80 2057
[12] Nicula R, Jianu A, Ponkraz U and Burkel E 2000 Phys. Rev. B 62 8844
[13] Sadoc A, Itie J P, Polian A, Kim J K and Kelton K F 2001 J. Phys. : Cond. Matt. 13 8527
[14] J Z Jiang, Gerward L and Olsen J S 2001 Appl. Phys. Lett. 79 2538
[15] Hasegawa M, Tsai A P and Yagi T 1999 Phil. Mag. Lett. 79 691
[16] Hasegawa M, Tsai A P, Kondo T, Yagi T and Kikegawa T 1999 J. Non-Crystal Solids 250-252 849
[17] Hasegawa M, Tsai A P and Yagi T 2000 Phil. Mag. A 80 1769
[18] Horn A P, Malzfeldt W, DiVincenzo D P, Toner J and Gambino R 1986 Phys. Rev. Lett. 57 1444
[19] Calvayrac Y, Quivy A, Bessiere M, Lefebvre S, Cornier-Quiquandon M and Gratias D 1990 J. Phys. France 51 417
[20] Tsai A P, Chen H S, Inoue A and Masumoto T 1991 Phys. Rev. B43 8782
[21] Nikura A, Tsai A P, Inoue A and Masumoto T 1994 Phil. Mag. Lett. 69 351
[22] Hasegawa M and Yagi T 2000 J. Crystal Growth 217 349
[23] Yagi T, Uchiyama Y, Akaogi M and Ito E 1992 Phys. Earth and Planet. Inter. 74 1
[24] Guryan C A, Goldman A I, Stephens P W, Hiraga K, Tsai A P, Inoue A and Masumoto T 1989 Phys. Rev. Lett. 62 2409