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The pressure-induced phase transition of Ga₂O₃

Baozhao Tu¹, Qiliang Cui^{1,3}, Peng Xu¹, Xin Wang¹, Wei Gao¹,
Chengxin Wang¹, Jing Liu^{1,2} and Guangtian Zou¹

¹ National Laboratory of Superhard Materials, Jilin University, Changchun 130023,
People's Republic of China

² BSRF, Institute of High Energy Physics, Academia Sinica, Beijing 100039,
People's Republic of China

E-mail: qiliangcui@yahoo.com.cn

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Abstract

In this paper, we investigate the pressure-induced structural transition of α -Ga₂O₃ powder by means of energy-dispersive x-ray diffraction (EDXD) measurements. The EDXD results show that, with increase of pressure, a new pressure-induced phase appears. The new tetragonal structure (β -Ga₂O₃) can remain stable over the pressure range (≤ 38 GPa) under study.

1. Introduction

Ga₂O₃ is a wide-band-gap ($E_g = 4.9$ eV) [1] compound which has long been known to exhibit both conduction and luminescence properties [2–4]. Nanoscale Ga₂O₃, which is made from Ga₂N, also been researched in depth. But its properties under high pressure have never been reported. In this paper, we report the properties of the pressure-induced phase transition of Ga₂O₃.

Ga₂O₃ can exist in four types; they are α -Ga₂O₃, β -Ga₂O₃, γ -Ga₂O₃ and ε -Ga₂O₃. The most stable one is α -Ga₂O₃, which is monoclinic. β -Ga₂O₃ and γ -Ga₂O₃ are harder materials. The β -type material has the tetragonal structure and the γ -type form shows the behaviour of a cubic structure.

2. Experiment

Our sample is white powder of Ga₂O₃. The XRD results under ambient pressure and temperature show that the sample is an α -Ga₂O₃ crystal. Figure 1 shows the energy-dispersive x-ray diffraction spectra of Ga₂O₃ at ambient pressure and temperature. By making calculations using the experimental data we can identify the sample as having monoclinic structure at ambient conditions and $a = 12.633$ Å, $b = 19.687$ Å, $c = 3.052$ Å, $\beta = 105.464^\circ$. The unit-cell volume is 731.50 Å³. (The data were calculated using the 'Powder X' software, which uses 'Treor90' to index the powder x-ray diffraction patterns.)

³ Author to whom any correspondence should be addressed.

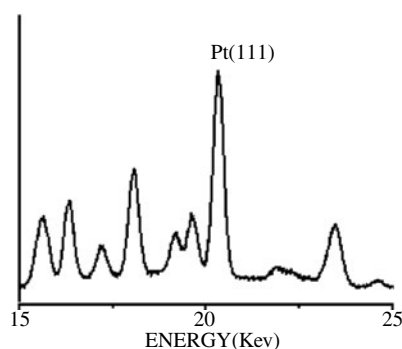


Figure 1. The energy-dispersive x-ray diffraction pattern of Ga_2O_3 under normal pressure.

A Mao–Bell-type diamond anvil cell (DAC) was used to generate high pressure. Using the cell, we carried out *in situ* high-pressure x-ray diffraction studies on Ga_2O_3 using synchrotron radiation. The whole experiment took place in the Institute of High Energy Physics, Academia Sinica, in Beijing. The padding material was L605 (stainless steel). The padding material had been hardened by application of 10 GPa pressure. The radius of the sample container is about 200 μm . The medium used to transfer pressure was a mixture of methyl alcohol, ethanol and water. Each spectrum was collected for 600–900 s. The position of the (111) diffraction peak of Pt and the formula $Ed (\text{keV nm}) = 0.619927/\sin \theta$ was used to determine an internal pressure standard. The diffraction angle $\theta = 8.244^\circ$.

3. Results and discussion

Figure 2 shows the spectra for energy-dispersive x-ray diffraction of Ga_2O_3 at various pressures. One observes that all the diffraction peaks shift to higher energy with increasing pressure. At about 2.25 GPa, we identified the peak between Pt(111) and Pt(222) as being induced by padding material. So we relocated the cell and the peak disappeared.

At about 13.3 GPa, peaks 1 and 2 disappear. New peaks (3, 6 and 7) appear. As the pressure gets larger, these peaks become ever clearer. They are stable over the pressure range (≤ 38 GPa) under study.

Figure 3 shows the d -spacing of Ga_2O_3 under various pressures. It shows clearly the transformations of the peaks. After 13.3 GPa, the slopes of these lines has changed. Line 5 is broken; so we think that the new peaks 4 and 5 are no longer related to the old structure: they relate to the new phase that appears. Because the slope after 13.3 GPa is smaller, we can assume that the new structure is harder. Because $\gamma\text{-Ga}_2\text{O}_3$ is definitely a harder material with cubic structure, we might think that Ga_2O_3 became $\gamma\text{-Ga}_2\text{O}_3$ after 13.3 GPa. But our calculations, with about 10% error, show that the new structure cannot be cubic. So the new structure is most probably tetragonal $\beta\text{-Ga}_2\text{O}_3$.

So we used the ‘PowerX’ software once again to process the data. We picked out the six strongest peaks at 37 GPa to index the powder x-ray diffraction patterns (see table 1).

The results from the software analysis show that the new structure is tetragonal with $a = 8.097 \text{ \AA}$, $b = 8.097 \text{ \AA}$ and $c = 10.062 \text{ \AA}$. This result also explains why the new structure is very close to cubic structure.

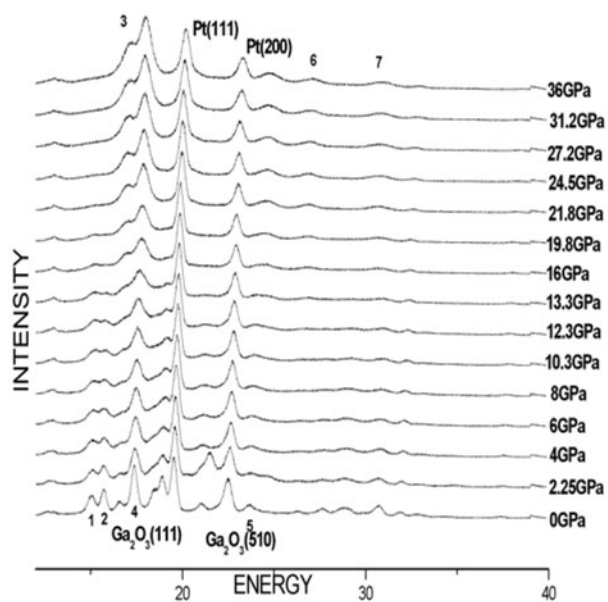


Figure 2. Energy-dispersive x-ray diffraction patterns of Ga₂O₃ under various pressures.

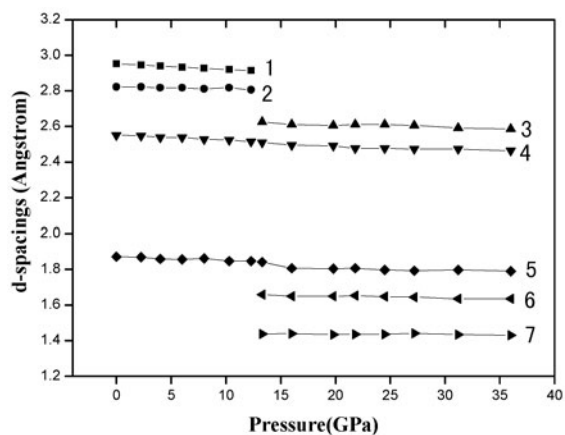


Figure 3. The *d*-spacing of Ga₂O₃ under various pressures.

Table 1. The six strongest peaks at 37 GPa.

<i>d</i> -spacing (Å)	Intensity
3.41	174
2.58	645
2.46	1000
2.19	813
1.90	428
1.78	241

4. Conclusions

The experiments show that, in the energy-dispersive x-ray diffraction patterns of Ga₂O₃, with increasing pressure, the old peaks disappear (at about 13.3 GPa) and new peaks appear. A structural transition becomes apparent. Monoclinic α -Ga₂O₃ turns into tetragonal β -Ga₂O₃. The new tetragonal structure (β -Ga₂O₃) can remain stable over the pressure range (≤ 38 GPa) of our research.

Acknowledgments

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