Powder x-ray diffraction of BaFe₂As₂ under hydrostatic pressure

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We measured the electrical resistivity of BaFe₂As₂ under high pressure using a modified-Bridgman anvilcell with Fluorinert, which resulted in the superconductivity with $T_c = 35$ K and $P_c = 3$ GPa.¹ On the other hand, Yamazaki reported that the pressurization using a cubic-anvil cell gives the maximum of $T_c = 17$ K at $P_c = 11$ GPa.² We suppose hydrostaticity influences not only the values of T_c and P_c but also the structure. In this study, single crystals of BaFe₂As₂, which were also used for the measurement of resistivity, were broken into powders to perform powder x-ray diffraction. The sample was pressurized up to 16.5 GPa using DAC with a helium gas at room temperature. The diffraction patterns show a tetragonal structure with a space group of I4/mmm in the whole pressure range. The pressurization of our sample does not make 109.47° of As-Fe-As angle. The difference between our result and other works on structure means that the pressure-induced structural-change in BaFe₂As₂ depends on the experimental condition.

¹F. Ishikawa *et al.*, Phys. Rev. B **79**, 172506 (2009).

²T. Yamazaki *et al.*, Phys. Rev. B **81**, 224511 (2010).