

*Identification of the atomic cluster of p-type Zn-Mg-Hf icosahedral quasicrystal*Hiroyuki Takakura¹, Ryosuke Kyojima¹¹Division Of Applied Physics, Faculty Of Engineering, Hokkaido University, Sapporo, Japan
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The structure of p-type Zn-Mg-Hf icosahedral quasicrystal (iQC) [1] has been analyzed by single-crystal X-ray diffraction within the framework of higher-dimensional structure analysis. The analysis revealed for the first time that the structure is isostructural to that of Cd-Yb iQC [2]. Thus the atomic cluster that characterizes the iQC structure is so-called Tsai-type, which is different from the Bergman-type that has been estimated from the structure analyses of related approximant crystals [3]. The structure refinements of Zn_{85.5}Mg₇Hf_{7.5} iQC based on the six-dimensional Cd-Yb iQC model [2] smoothly converged with the reliability factor of 0.096 using symmetrically inequivalent 2946 reflections and 290 refined parameters. It became apparent that Zn occupies the atomic sites of Cd, and Mg/Hf occupies those of Yb. This contrasts with Cd-Mg-Yb iQCs, where Cd is replaced with Mg when varying their Mg concentrations. The authors would like to thank Dr. Y. Matsushita and Mr. A. Sato for their assistance during the X-ray diffraction measurement at NIMS. This work was supported by JSPS KAKENHI Grant Number JP15K04659.

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