Thesis Title The Development of Indexing Reflections of Crystals in Monoclinic

System

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Abstract

The software using the Trial and Error Method with various parameter was created for indexing the crystal plane (hkl.) of crystal in monoclinic system, the low symmetry of which made the indexing very difficult and complicated. Indexing method was studied in some systems such as cubic, tetragonal and orthorombic. Then the indexing on the monoclinic system was applied by using Visual Basic Program and the unit cell dimensions a, b, c and β were calculated. The Visual Basic Program was designed to be easy for using by graphic commands. This program was tested by using the powder diffraction data from JCPDS (Joint Committee Powder Diffraction Society) with input data for this program at $\sin^2\theta_{obs}$, θ was the Bragg's angle. Then $\sin^2\theta_{obs}$ was compared with $\sin^2\theta_{ob}$ that calculated by using a, b, c, β , h, k and 1 related to the $\sin^2\theta$ in monoclinic system. The difference between $\sin^2\theta_{ob}$ and $\sin^2\theta_{obs}$ was defined to be not more than \pm 0.00050. The 80 samples were used to test the program and 70 percent of the test samples were indexed successfully. The others that had Miller planes except set (101), $(10\overline{1})$, (202), $(20\overline{2})$, (303), $(30\overline{3})$ and set (111), $(11\overline{1})$, (222), $(22\overline{2})$, (333), $(33\overline{3})$ could not be indexed because of their plane (hkl) groups were not covered by the program.