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Oxidation States of Trace Elements in Synthetic Corundum

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Abstract : Natural corundum occurs in various colors due to impurities or trace elements in its structure. Sapphire and ruby are essentially the same mineral, corundum, but valued differently due to their red and blue varieties, respectively. Color is one of the critical factors used to determine the value of natural and synthetic corundum. Despite the abundance of research on impurities in natural corundum, little is known about trace elements in synthetic corundum. This project thus aims to quantify trace elements and identify their oxidation states in synthetic corundum. A total of 15 corundum samples in red, blue, and yellow, synthesized by melt growth process, were first investigated by X-ray diffraction (XRD) analysis to determine the composition. Electron probe micro-analyzer (EPMA) was used to identify the types of trace elements. Results confirm that all synthetic corundums contain crystalline Al_2O_3 and a wide variety type of trace element, particularly Cr, Fe, and Ti. In red, yellow, and blue corundums respectively. To further determine their oxidation states, synchrotron X-ray absorption near edge structure spectrometry (XANES) was used to observe absorbing energy of each element. XANES results show that red synthetic corundum has Cr^{3+} as a major trace element (62%). The pre-edge absorption energy of Cr^{3+} is at 6001 eV. In addition, Fe^{2+} and Fe^{3+} are dominant oxidation states of yellow synthetic corundum while $Ti^{3+}$and Ti^{4+} are dominant oxidation states of blue synthetic corundum. the average absorption energy of Fe and Ti is 4980 eV and 7113 eV respectively. The presence of Fe^{2+}, Fe^{3+}, Cr^{3+}, Ti^{3+}, and Ti^{4+} in synthetic corundums in this study is governed by comparison absorption energy edge with standard transition. The results of oxidation states in this study conform with natural corundum. However yellow synthetic corundums show difference oxidation state of trace element compared with synthetic in electron spin resonance spectrometer method which found that Ni^{3+} is a dominant oxidation state.

Keywords : corundum, trace element, oxidation state, XANES technique
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