Yellow and colourless anorthite megacrysts from Hakone volcano: Structural controls on colouration

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Anorthite megacrysts from Hakone volcano, Japan with about 94 mol% of $CaAl_2Si_2O_8$ component contain about 0.4 wt% of FeO. It is known that Fe^{2+} enters anorthite through the coupling substitution (Fe^{2+} + Si^{4+}) for 2 Al^{3+}. On the other hand, simple substitution of Fe^{3+} for Al^{3+} in K-feldspar is common and forms the $KFeSi_3O_8$ end-member [1]. In addition, according to stoichiometric calculations based on the data for anorthite megacrysts from island arc, Fe^{2+} can partially replace Ca^{2+} on the M-site [2]. Thus, iron can enter feldspar in either trivalent or divalent form. In the Hakone district, there are two types of anorthite megacryst which are coloured yellow and colourless. Substitution of Fe^{3+} for Al in tetrahedral sites produces a yellow colour because of absorption bands in the blue region [3]. Consequently, it is suggested that ferric iron may partialy occpy the T-site in the feldspar structure of the megacryst coloured yellow.

Preliminary analysis by XPS had shown that iron in the yellow megacryst was ferric [4]. Crystal structures of the above yellow and colourless anorthite megacrysts were refined from single crystal diffraction data in space group *P*-1 and *I*-1 respectively. Average T-O bond distances for both megacrysts suggested that Al/Si distributions in the T-site were highly ordered. In particular, the T_1(0z00)-site in the yellow sample, the T-O bond distance was slightly longer and the isotropic temperature factor was just smaller than the other Al-sites. Judging from the compositional data (EPMA) and the structural evidence (XRD) it seems reasonable for ferric iron to enter T-site in the yellow one, and for ferrous iron into the M-site of the colourless sample. These results imply that a somewhat large and heavy cation occupies the T_1(0z00)-site, namely, partial replacement of Al^{3+} by Fe^{3+}. Thus, the colouration in the yellow anorthite megacryst was confirmed structurally. The outcome of the site preference of iron is heavily influenced by a vast variety of physico-chemical conditions. Therefore, determination of the site and the valence state of iron does not only provide an answer for the colouration but can give useful insight into the conditions under which these anorthite megacrysts form.

[1] Petrov & Hafner (1988) *American Mineralogist,* **73**, 97-104. [2] Kimata *et al*. (1994) *Mineralogical Magazine,* **59**, 1-13. [3] Hofmeister & Rossman (1983) *Reviews in Mineralogy,* **2**, 271-280. [4] Matsui *et al*. (2015, in preparation).