Al-Si ordering in the incommensurately modulated structures of *e*-plagioclases

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Plagioclase feldspars, the solid solution between albite ($NaAlSi_3O_8$) and anorthite ($CaAl_2Si_2O_8$), are the most abundant group of minerals in the Earth's crust. The crystal structure of feldspar is constructed by a three-dimensionally interconnected Al-Si tetrahedral framework, with larger cations (Ca, Na and K) filling the cavities inside. The coupled substitution between Na+Si and Ca+Al in the plagioclase solid solution results in a continuous variation in the Al/Si ratio of the composition, which is believed to be the reason for the dramatically different ordering patterns in the tetrahedral framework. The ordering pattern in the incommensurately modulated structures of *e*-plagioclase (characterized by the satellite diffraction peak called *e*-reflections) are the most complicated and intriguing.

To bettering understand the Al-Si ordering in the tetrahedral framework, the incommensurately modulated structure of an iridescent labradorite sample (7147A) from Labrador, Canada is refined with single-crystal neutron diffraction data for the first time. As a comparison, the disordered structure of a volcanic phenocryst plagioclase sample (MXCG) from Casas Grandes, Mexico is also studied with neutron diffraction. The Al occupancy in the well-ordered structure of sample 7147A correlates strongly with the size of the tetrahedral sites. However, in the disordered structure of sample MXCG, the Al occupancy difference between T_1o and T_1m sites are not significant, even though the T_1o site is obviously larger than the T_1m site. The M site of the structure refined from neutron diffraction data also show some interesting features that's not observable from X-ray diffraction data. The discrepancy between the tetrahedra size and Al occupancy in the structure of sample MXCG indicates that the Al-Si ordering is driven by the tetrahedra sized difference caused by the framework collapsing and distortion upon cooling, but not the other way around. The rigid-unit-mode (RUM) analysis of the disordered structure shows that the satellite peaks initiate around the highest frequencies (Anti-Rigid Unit Mode or ARUM) instead of the lowest ones (RUM), which suggests the structural modulation is to accommodate the internal strain generated by the local ordering of Al and Si in the framework.