Order-Disorder in K-Feldspars by ^{27}Al MAS NMR at 19.6 T

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Introduction

$KAlSi_3O_8$ structure consists of a 3D network of tetrahedral cations with a variety of schemes of local Si/Al order. Two phases have been recognized: a monoclinic *C*2/m phase has two sites (T_1 and T_2), a triclinic C-1 phase with four sites (T_1o, T_1m, T_2o, T_2m). Si/Al order has been traditionally evaluated from T-O averages distanced from X-ray diffraction data. However, local symmetry and order degree data from X-ray diffraction are not consistent with those values obtained by means of ^{29}Si MAS NMR [1,2]. The central transition of ^{27}Al MAS NMR spectra at 11.7 T have not resolved different lattice sites [1] because of quadrupolar broadening and also similar δ_{iso} values for the distinct sites. In this work, ^{27}Al MAS NMR satellite-transition (SATRAS) spectra were obtained using a 19.6 T spectrometer to describe the local structure along the order-disorder series.

Experimental

Samples were collected in National Museum of Natural Science (Madrid, Spain) and Muséum National d'Histoire Naturelle (Paris, France). Solid-state 27Al MAS NMR spectra were obtained with an 830 MHz (19.6 T) ultra narrow bore (31 mm bore size) superconducting magnet with a 10 kHz MAS probe, using a 2 mm rotor, recycle delay of 5 s at the National High Magnetic Field Laboratory (Tallahassee, FL). Quadrupolar parameters were evaluated using WINFIT program from Bruker.

Results and Discussion

Figure 1 present the ^{27}Al spectra of the two end-member structures of the Si/Al order-disorder series. Fig. 1a is the SATRAS spectrum of a triclinic crystal with maximum order, the central transition shown in Fig. 1b. Al atoms are occupying only the T_1o site with δ_{iso} at 58.9 ppm. A C_Q quadrupole coupling constant of 3.3 MHz and η asymmetry parameter of the EFG of 0.2 was evaluated from both the satellite and central transitions. When disorder progresses a signal with δ_{iso} at ~61 ppm appears and the SATRAS profile becomes broad. Fig. 1c is the SATRAS spectrum of a monoclinic crystal with maximum disorder being Fig. 1d its central transition. Al atoms are occupying the two T_1 and T_2 sites that can not be described by particular quadrupolar parameters neither η asymmetry parameters, indicating a wide distribution of the quadrupole interaction.

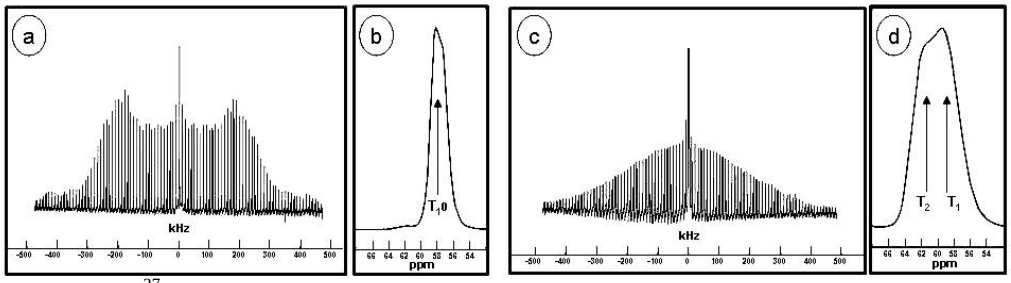

Figure. 1. ^{27}Al MAS NMR spectra at 19.6 T of order-disorder K-feldspar end-members.

Conclusion

When the crystalline sites of disordered K-feldspars are analyzed by quadrupolar nucleus, a "site distribution" emerges because of a EFG distribution. Electronic disorder coexisting along with atomic disorder is described for the first time.

Acknowledgements

LSM thanks NHMFL and NSF for support, and also CIEMAT (grant number FIS2007-61823) for travel expenses.

References

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