1 **Phase relations of the nepheline-kalsilite system: X-ray diffraction and**
2 **Mössbauer spectroscopy**

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Abstract

The crystalline solutions in the nepheline-kalsilite (NaAlSiO_4 - KAlSiO_4) system form an important group rock-forming tectosilicates, which have significant applications for materials science and implications for the geology field. The present studies on phase relations of the Fe-free and Fe-bearing nepheline-kalsilite systems have demonstrated that 10 mol % of Fe^{3+} substitution in Al^{3+} does not affect the phase relations of the solid solutions but causes the increase of lattice parameters. Analysis of the Mössbauer spectra has indicated that low-temperature carnegieite, low-temperature nepheline, and orthorhombic KAlSiO_4 O1 phases in the $\text{Na}(\text{Al}_{0.9}\text{Fe}_{0.1})\text{SiO}_4$ - $\text{K}(\text{Al}_{0.9}\text{Fe}_{0.1})\text{SiO}_4$ system only have one doublet assigned to high-spin Fe^{3+} with tetrahedral coordination, which means the doped Fe^{3+} cations occupy the Al^{3+} sites forming tetrahedrons with surrounding oxygen atoms based on charge balance.

Keywords: nepheline-kalsilite system; phase relations; X-ray diffraction; Mössbauer spectroscopy

1. Introduction

The phase relations in the nepheline-kalsilite (NaAlSiO_4 - KAlSiO_4) system at subsolidus temperatures have been investigated systematically [1-4]. The phase relationships of this solid solution system are very complicated, especially in the potassium-rich part of the phase diagram. The existence of a relatively large gap in solid solubility between nepheline and kalsilite has been demonstrated by Tuttle and Smith [1], and it is similar to the solvus between albite and orthoclase [5]. Eleven crystalline phases have been reported in the nepheline-kalsilite system, and there are high- and low-temperature carnegieite (high- and low-Cg), high- and low-temperature nepheline (Ne_h and Ne), trinepheline (tri-Ne), tetrakalsilite (H_4), kalsilite (Ks), kaliophilite and disordered kaliophilite (Kp), orthorhombic KAlSiO_4 O1 and O2 phases [1, 2, 6-8]. The high-Cg phase with a cubic symmetry is stable at above 1250 °C and inverts to the low-Cg phase with an orthorhombic structure at lower temperatures. All other phases (Ne, tri-Ne, H_4 , Ks, and Kp phases) have hexagonal

symmetry except for Ne_h , orthorhombic KAlSiO_4 O1 and O2 phases, which are orthorhombic structure. Orthorhombic KAlSiO_4 O1 phase actually has a monoclinic symmetry with $\beta \approx 90^\circ$ (so called pseudo-orthorhombic symmetry), thus it generally was identified as ‘orthorhombic KAlSiO_4 -O1’ or ‘orthorhombic KAlSiO_4 -O1 (low temperature)’ in previous studies [1, 2, 9, 10]. Those natural and synthetic phases in the nepheline-kalsilite system are all tectosilicates, whose crystal structures are composed of three-dimensional frameworks of SiO_4 and AlO_4 tetrahedrons linking by shared corners, with Na^+ and K^+ as interstitial charge-balancing cations.

Studies on thermal expansion of the nepheline-kalsilite solid solutions with various K^+/Na^+ ratios indicate that nepheline expansion is relatively high and little affected by composition, whereas kalsilite expansion is lower but affected to a significant degree by K^+/Na^+ ratio [11]. Chemical compositions of those solutions may also vary by the coupled $\square + \text{Si}^{4+} \leftrightarrow \text{K}^+/\text{Na}^+ + \text{Al}^{3+}$ substitution (where $\square$ represents vacancy), which has been reported in both natural and synthetic nepheline-kalsilite solid solutions [12-15]. In the generalized formula $(\text{K},\text{Na})_{1-x}\square_x\text{Al}_{1-x}\text{Si}_{1+x}\text{O}_4$, “x” characterizes the “excess silicon” per four oxygen ions, which may affect thermodynamic, phase equilibrium, and crystal chemical behavior of the nepheline-kalsilite system [12, 13, 16, 17]. High-Si series relative to stoichiometric $\text{Al} : \text{Si} = 1 : 1$ exhibit lower mixing enthalpies and produce a lower critical temperature of the solvus than series containing less silicon [12, 13, 16, 17]. Additionally, chemical compositions of the natural specimens in the nepheline-kalsilite system vary systematically not only in Na^+/K^+ ratio but also in Ca^{2+} and vacancy contents due to $\square + \text{Ca}^{2+} \leftrightarrow 2\text{K}^+/\text{Na}^+$ substitution [13]. The substitution of Ca^{2+} in the alkali sites was found to increase substantially enthalpies of K-Na mixing and also to increase the critical temperature of the solvus [13]. The thermodynamic and phase behavior of phases in the nepheline-kalsilite system are related to structural strain associated with the entrance of K^+ into the smaller alkali crystallographic sites in the nepheline group phases [17].

The synthetic analogs in the NaAlSiO_4 - KAlSiO_4 binary have long been of interest to ceramists and materials scientists. The nepheline-kalsilite group phases

have been demonstrated to show an excellent and highly improved oxidation activity of carbon toward diesel soot combustion [18], and also can be used as a heterogeneous catalyst for biodiesel production [19]. In addition, the polymorphs of NaAlSiO₄, including low-Cg, Ne_h, and Ne phases, can be excellent candidate phosphor host materials for light emitting diodes. Those phases are made of open, three dimensional frameworks of SiO₄ and AlO₄ tetrahedra, which can accommodate rare earth and transition metal ions, such as Eu²⁺ [20], Dy³⁺ [21], Mn²⁺ [22], and Fe³⁺ [23].

Although the phase diagram of the nepheline-kalsilite system involving in composition and temperature has been investigated systematically so far, the Fe-bearing solid solutions have not been studied yet. Since, the natural specimens in the nepheline-kalsilite system contain some amount irons [15, 24], the valence and spin states of irons in the solid solutions may potentially affect their thermodynamic behavior, physical and chemical properties. These motivate us to thoroughly investigate the phase relations of the Fe-free and Fe-bearing nepheline-kalsilite systems by means of powder X-ray diffraction (XRD). As well as, the valence and spin states of irons in Fe-bearing nepheline-kalsilite systems have been elucidated by Mössbauer spectroscopy (MS).

2. Experiments

Two groups of samples, NaAlSiO₄-KAlSiO₄ and Na(Al_{0.9}Fe_{0.1})SiO₄-K(Al_{0.9}Fe_{0.1})SiO₄ systems, were synthesized from reagent grade chemicals by standard solid state reaction. For the NaAlSiO₄-KAlSiO₄ system, samples with chemical compositions of 100%NaAlSiO₄-0%KAlSiO₄ (100Na-0K) in mole ratio, 80Na-20K, 60Na-40K, 40Na-60K, 80Na-20K, and 0K-100Na were synthesized, while for Na(Al_{0.9}Fe_{0.1})SiO₄-K(Al_{0.9}Fe_{0.1})SiO₄ system, 100%Na(Al_{0.9}Fe_{0.1})SiO₄-0%K(Al_{0.9}Fe_{0.1})SiO₄ (100Na-0K-Fe), 80Na-20K-Fe, 60Na-40K-Fe, and 0Na-100K-Fe were synthesized. A mixture of Na₂CO₃/K₂CO₃, Al₂O₃, and SiO₂ with a mole ratio of 1.02 : 1.00 : 1.00 were ground together with ethanol in an agate mortar. The small additional amount (2 mol %) of Na₂CO₃/K₂CO₃

relative to the stoichiometric mole ratio (1 : 1 : 1) was added in the starting materials, since a small amount of Na₂O or K₂O may evaporate during the long time annealing. While 10 mol % of the Al₂O₃ in the starting mixtures was substituted by Fe₂O₃ for the Na(Al_{0.9}Fe_{0.1})SiO₄-K(Al_{0.9}Fe_{0.1})SiO₄ system. The mixtures were compressed into disks and sintered in air at 1300 °C for 24 hours.

The crystal structures of both Fe-free and Fe-bearing samples were characterized by powder XRD using a Bruker AXS D8-Focus diffractometer with Cu K α radiation (λ = 1.5406 Å). The XRD patterns were refined using the GSAS program to obtain unit-cell lattice parameters [25]. Mössbauer spectra of the Fe-bearing samples for the Na(Al_{0.9}Fe_{0.1})SiO₄-K(Al_{0.9}Fe_{0.1})SiO₄ system were collected at ambient conditions using a ⁵⁷Co in Rh point source in transmission geometry. The obtained Mössbauer spectra were analyzed using the program MossA to obtain electrical configurations and local environment of irons in the Fe-bearing nepheline-kalsilite system [26].

3. Results and discussion

XRD patterns of the Fe-free samples in the NaAlSiO₄-KAlSiO₄ system are shown in Fig. 1. As seen in Fig. 1(a), the diffraction peaks of 100Na-0K sample with a chemical composition of NaAlSiO₄ were indexed to low-Cg phase (orthorhombic, *Pb*2₁*a*, Z=8), and XRD patterns of both 80Na-20K and 60Na-40K samples were assigned to low-temperature Ne phase (hexagonal, *P*6₃, Z=8). In Fig. 1(b), the 0Na-100K sample with a composition of KAlSiO₄ end member has a crystal structure of orthorhombic KAlSiO₄ O1 phase (monoclinic, *P*2₁, Z=12) [9]. The label ‘O1’ has been quoted in this study. While XRD patterns in Fig. 1(b) show that two different phases coexist in the 40Na-60K and 20Na-80K samples, Ne and Ks phases (Ks: hexagonal, *P*6₃, Z=2) for the 40Na-60K sample; Ks and O1 phases for the 20Na-80K sample. The phase relations of the Fe-free nepheline-kalsilite system synthesized at 1300 °C are in good agreement with the results of Tuttle and Smith [1].

For the Fe-bearing nepheline-kalsilite (Na(Al_{0.9}Fe_{0.1})SiO₄-K(Al_{0.9}Fe_{0.1})SiO₄) system, we have synthesized four samples: 100Na-0K-Fe, 80Na-20K-Fe, 60Na-40K-Fe, and 0Na-100K-Fe, and their XRD patterns are shown in Fig. 2. The

100Na-0K-Fe sample has a crystal structure of low-Cg phase, XRD patterns of 80Na-20K-Fe and 60Na-40K-Fe samples are assigned to Ne phase, and the 0Na-100K-Fe sample is O1 structure. To compare with the NaAlSiO₄-KAlSiO₄ system, the Fe-bearing samples in the Na(Al_{0.9}Fe_{0.1})SiO₄-K(Al_{0.9}Fe_{0.1})SiO₄ system have the same crystal structures as those of Fe-free samples, and it indicates the substitution of 10 mol % Fe in Al does not affect phase relations of the nepheline-kalsilite system.

Lattice parameters of the phases in both NaAlSiO₄-KAlSiO₄ and Na(Al_{0.9}Fe_{0.1})SiO₄-K(Al_{0.9}Fe_{0.1})SiO₄ systems were obtained by a full-profile model refinement (Le Bail method) implemented in the GSAS program (Tab. 1). For the monoclinic O1 phase in the samples, the refined β (90° ~ 91°) is close to 90° and has not been listed in Tab. 1. For further discuss the composition-dependent relations among these phases, their volumes per formula in both Fe-free and Fe-bearing nepheline-kalsilite system have been calculated and plotted in Fig. 3 for comparison. The Fe-bearing phases have larger lattice parameters than the Fe-free phases, as the ionic radius of doped Fe in tetracoordinated sites (either Fe²⁺ or Fe³⁺, further discussed in next paragraph) ($R(\text{Fe}^{2+}) = 0.77 \text{ \AA}$ and $R(\text{Fe}^{3+}) = 0.63 \text{ \AA}$) is larger than that of Al³⁺ ($R(\text{Al}^{3+}) = 0.53 \text{ \AA}$) [27]. Additionally, volumes per formula of phases exhibit an increasing trend with increasing the amount of KAlSiO₄, which is attributed to the larger ionic radius of K⁺ than Na⁺.

Mössbauer spectra of the Fe-bearing samples (100Na-0K-Fe, 80Na-20K-Fe, 60Na-40K-Fe, and 0Na-100K-Fe) in the Na(Al_{0.9}Fe_{0.1})SiO₄-K(Al_{0.9}Fe_{0.1})SiO₄ systems are shown in Fig. 4. The spectra of four Fe-bearing samples (low-Cg, Ne, and O1 phases) were well-fitted using one doublet of iron and the obtained hyperfine parameters were listed in Tab. 2. The doublets of iron in the Fe-bearing low-Cg, Ne, and O1 phases have isomer shift (IS) of 0.10~0.12 mm/s (relative to α -Fe) and quadrupole splitting (QS) of 0.59~0.62 mm/s (Tab. 2). Due to preferred orientation of the samples, the area and width ratios between two lines (W21 and A21) of the double exhibit small deviations from 1 (W21: 1.0~1.1; A21: 0.9~1.2). Based on the derived hyperfine parameters and previous studies [28], the doublets can be assigned to

high-spin Fe^{3+} with tetrahedral coordination in the Fe-bearing low-Cg, Ne, and O1 phases (Fig. 5).

The site assignment of the high-spin Fe^{3+} in the low-Cg, Ne, and O1 phases can be reconciled with their structures. The nepheline-kalsilite system has a general formula of ABCO_4 for the low-Cg, Ne, Ks, and O1 phases. As shown in Fig. 5, atom ball labeled A represents large monovalent cation (K^+ or Na^+), B represents small-sized Al^{3+} or Fe^{3+} , and C stands for Si^{4+} . For those four structures, cations in B and C sites coordinate with surrounding four oxygen atoms to form tetrahedrons and they distribute orderly on alternating tetrahedrons, so that every BO_4 tetrahedron is coordinated to four CO_4 tetrahedra by sharing corners (O atoms) and vice versa. The $[\text{BCO}_4]$ tetrahedral frameworks of those four phases are topological variants of tridymite structure. The K^+ or Na^+ cations are located in the space of the framework of tetrahedrons. The four phases in Fig. 5 have similar tetrahedral frameworks, but a different arrangement of tetrahedrons. According to the results of MS, low-Cg, Ne, and O1 phases only have one doublet of high-spin Fe^{3+} , which indicates the doped Fe^{3+} occupies the Al^{3+} site forming tetrahedron with surrounding oxygen atoms based on the principle of charge balance.

4. Conclusions

In summary, the solid solutions in the $\text{Na}(\text{Al}_{0.9}\text{Fe}_{0.1})\text{SiO}_4$ - $\text{K}(\text{Al}_{0.9}\text{Fe}_{0.1})\text{SiO}_4$ system have the same phase relations as those in the NaAlSiO_4 - KAlSiO_4 system, and it indicates the substitution of 10 mol % Fe^{3+} in Al^{3+} does not affect the crystal structures of solid solutions. The obtained lattice parameters of the Fe-bearing phases are larger than those of Fe-free phases, as the ionic radius of doped Fe^{3+} is larger than that of Al^{3+} . In the $\text{Na}(\text{Al}_{0.9}\text{Fe}_{0.1})\text{SiO}_4$ - $\text{K}(\text{Al}_{0.9}\text{Fe}_{0.1})\text{SiO}_4$ system, the doped high-spin Fe^{3+} occupy the tetrahedral Al^{3+} sites in low-Cg, Ne, and orthorhombic KAlSiO_4 O1 phases.

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Figure Captions

Figure 1 XRD patterns of the 100Na-0K, 80Na-20K, 60Na-40K, 40Na-60K, 80Na-20K, and 0K-100Na samples in the NaAlSiO₄-KAlSiO₄ system.

Figure 2 XRD patterns of the 100Na-0K-Fe, 80Na-20K-Fe, 60Na-40K-Fe, and 0Na-100K-Fe samples in the Na(Al_{0.9}Fe_{0.1})SiO₄-K(Al_{0.9}Fe_{0.1})SiO₄ system.

Figure 3 Volumes per formula of the phases in the NaAlSiO₄-KAlSiO₄ and Na(Al_{0.9}Fe_{0.1})SiO₄-K(Al_{0.9}Fe_{0.1})SiO₄ system. The solid circles stand for phases in the Fe-free system and the open circles represent phases in the Fe-bearing system. Black: low-Cg phase; red: Ne phase; blue: Ks phase; orange: O1 phase.

Figure 4 Mössbauer spectra of the 100Na-0K-Fe, 80Na-20K-Fe, 60Na-40K-Fe, and 0Na-100K-Fe samples in the Na(Al_{0.9}Fe_{0.1})SiO₄-K(Al_{0.9}Fe_{0.1})SiO₄ system. Asterisks: experimental data; orange lines: calculated results.

Figure 5 Crystal structures of the phases in the nepheline-kalsilite system: (a) low-temperature carnegieite phase (low-Cg: *Pb2₁a*, Z=8), (b) low-temperature nepheline phase (Ne: *P6₃*, Z=8), (c) kalsilite phase (Ks: *P6₃*, Z=2), and (d) orthorhombic KAlSiO₄ O1 phase (O1: *P2₁*, Z=12). Atom ball labeled A represents K⁺ or Na⁺, B represents small-sized Al³⁺ or Fe³⁺, and C stands for Si⁴⁺.

Table 1 Lattice parameters of the phases in the NaAlSiO₄-KAlSiO₄ and Na(Al_{0.9}Fe_{0.1})SiO₄-K(Al_{0.9}Fe_{0.1})SiO₄ systems.

Filename	Phase	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	<i>V</i> (Å ³)
100Na-0K	low-Cg (<i>Pb</i> 2 ₁ <i>a</i>)	10.163(2)	13.950(3)	5.123(1)	726.3(4)
80Na-20K	Ne (<i>P</i> 6 ₃)	9.9858(3)	9.9858(3)	8.3533(3)	721.37(4)
60Na-40K	Ne	10.0545(2)	10.0545(2)	8.4063(3)	735.96(3)
40Na-60K	Ne	10.0523(3)	10.0523(3)	8.4079(3)	735.79(4)
	Ks (<i>P</i> 6 ₃)	5.1375(1)	5.1375(1)	8.6232(5)	197.11(1)
20Na-80K	Ks	5.2154(6)	5.2154(6)	8.5902(6)	202.35(4)
	O1 (<i>P</i> 2 ₁)	15.3606(4)	8.8876(2)	8.4823(3)	1157.81(4)
0Na-100K	O1	15.6356(3)	8.9653(3)	8.5491(3)	1180.80(5)
100Na-0K-Fe	low-Cg	10.2654(4)	14.0459(6)	5.1621(2)	744.30(4)
80Na-20K-Fe	Ne	9.9977(2)	9.9977(2)	8.3777(3)	725.20(3)
60Na-40K-Fe	Ne	10.0638(3)	10.0638(3)	8.4126(4)	737.87(4)
0Na-100K-Fe	O1	15.6464(7)	9.0417(4)	8.5529(3)	1209.97(6)

Table 2 Hyperfine parameters including isomer shift (IS), quadrupole splitting (QS), and the ratios of the line widths (W21) and areas (A21) for Fe³⁺ doublets in the phases in the Na(Al_{0.9}Fe_{0.1})SiO₄-K(Al_{0.9}Fe_{0.1})SiO₄ system.

Filename	Phase	IS (mm/s)	QS (mm/s)	W21	A21
100Na-0K-Fe	low-Cg	0.12(1)	0.62(1)	1.1(1)	1.0(1)
80Na-20K-Fe	Ne	0.10(1)	0.59(1)	1.2(1)	1.2(1)
60Na-40K-Fe	Ne	0.11(2)	0.60(1)	1.1(1)	1.0(2)
0Na-100K-Fe	O1	0.10(2)	0.61(1)	1.0(1)	0.9(2)

Figure1

Figure2

Figure3

Figure4

Figure5

(a) low-Cg phase ($Pb2_1a$)

(c) Ks phase ($P6_3$)

(b) Ne phase ($P6_3$)

(d) O1 phase ($P2_1$)