Study on the Thermal Stability of the Na$_2$UF$_8$ Complex in the Argon Atmosphere

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ABSTRACT: The Na$_2$UF$_8$ complex is an important intermediate compound in the purification of UF$_6$ by the adsorption-desorption process during fluoride volatility of the spent nuclear fuel, and its decomposition is seriously affected by temperature and atmosphere. In this study, the thermal stability of Na$_2$UF$_8$ in the argon atmosphere was investigated by the in situ Raman spectroscopy. The decomposition products of Na$_2$UF$_8$ at different temperatures were systematically determined by X-ray diffraction spectroscopy and X-ray absorption fine structure spectroscopy. The results indicated that Na$_2$UF$_8$ on the NaF sorbent was stable under 300 °C in the argon atmosphere, and it started to decompose into UF$_6$ and NaF rapidly when the temperature was above 300 °C. Meanwhile, a small amount of Na$_2$UF$_8$ was converted to Na$_3$UF$_7$, and it was stable in the temperature range from 350 to 450 °C. The decomposition mechanism of the Na$_2$UF$_8$ and the formation mechanism of Na$_3$UF$_7$ on the NaF sorbent were speculated according to the experimental results.

INTRODUCTION

In recent years, the Generation IV reactor systems, with better economy, safety, and sustainability, represented by the molten salt reactor, fast reactor, supercritical water reactor, and very high-temperature reactor, have received much attention in worldwide.$^{1}$ Because of the high burn-up or special fuel type of such reactors, the traditional aqueous reprocessing technologies are not satisfactory for the treatment of the spent nuclear fuel. With the advantages of high radiation resistance, compact facilities, less generation of waste, and so forth, pyroprocessing technologies have been considered as the best choice to treat high burn-up spent fuel,$^{2}$ and the fluoride volatility process (FVP), based on the different volatilities between uranium hexafluoride (UF$_6$) and fission product fluoride, has been regarded as a promising pyroprocessing technology for separating uranium from the spent nuclear fuel.$^{3–5}$

The FVP mainly includes the fluorination of uranium compounds and the purification of the UF$_6$ product. As the most widely used adsorption material in the purification of the UF$_6$ product, the NaF sorbent can selectively remove impurities from UF$_6$ through adsorption and desorption processes. The Na$_2$UF$_8$ complex forms during the adsorption of UF$_6$ on NaF sorbent, and the complex can decompose reversibly to UF$_6$ and NaF with the increase of the temperature. This reversible reaction between UF$_6$ and NaF is of great significance for the separation of the volatile impurities from the UF$_6$ product.$^{6–9}$ Our previous study indicated that Na$_2$UF$_8$ was stable in anhydrous environment, and the obvious desorption of UF$_6$ from NaF sorbent occurred when the temperature exceeded 200 °C with a maximal desorption rate of UF$_6$ at 330 °C. We also found that the desorption behavior of UF$_6$ from the NaF sorbent in the fluorine atmosphere was similar to that in the argon atmosphere, while the amount of the uranium residue on the NaF sorbent after desorption in the argon atmosphere (1.68 mg U/g NaF) was significantly larger than that in the F$_2$ atmosphere (0.006 mg U/g NaF).$^{7}$ Cathers et al.$^{10}$ speculated that the uranium residue on the NaF sorbent was the nonvolatile NaF–UF$_5$ complex when the Na$_2$UF$_8$ complex was heated to 200–450 °C in nitrogen, and the NaF–UF$_5$ complex was further converted into the NaF–UF$_4$ complex when the temperature was above 450 °C. By dissolving and analyzing the spent NaF from sorption columns of Chemical Combine, Gromov et al.$^{11}$ proposed that Na$_2$UF$_8$ (UF$_6$·2NaF) was decomposed into UF$_6$ and NaF directly in the range of 300–400 °C, and it could be transformed into Na$_3$UF$_7$ (UF$_5$·2NaF) in the range of 350–500 °C and then be further converted into Na$_3$UF$_7$ (UF$_2$·2NaF) when the temperature increased to 500–600 °C. Above off-line analysis results indicated that the decomposition of the Na$_2$UF$_8$ complex in...
The inert atmosphere would lead to the formation of the uranium residue on the NaF sorbent, and the temperature also had an important influence on the chemical form of the uranium residue.

The total desorption of UF₆ from the NaF sorbent is very important for the recovery of U and the reuse of NaF. In order to elucidate the mechanism of the formation of the uranium residue on the NaF sorbent, in situ Raman spectroscopy, a very useful in situ nondestructive assay surface characterization method was used to monitor the real-time and dynamic microstructure change of Na₂UF₈ in the decomposition process in argon at different temperatures. Furthermore, the chemical morphology and the coordination structure of the uranium residue on the NaF sorbent were determined by X-ray diffraction spectroscopy (XRD) and X-ray absorption fine structure spectroscopy (XAFS).

**RESULTS AND DISCUSSION**

**Effect of Temperature on Decomposition Behavior of the Na₂UF₈ Complex.** The Na₂UF₈ complex is an important intermediate in UF₆ purification processes based on adsorption and desorption on the NaF sorbent and temperature plays an important role in its decomposition behavior. In order to study the decomposition behavior of the Na₂UF₈ complex and formation mechanism of the uranium residue on the NaF sorbent in argon, the in situ Raman spectroscopic analysis technique was used to monitor the stability of Na₂UF₈ on the NaF sorbent.

As shown in Figure 1a, there existed several peaks locating at 170, 286, 306, 345, 375, 411, and 609 cm⁻¹ at room temperature, which was consistent with our previous work.⁹ The characteristic vibrational frequency at 609 cm⁻¹ was assigned to the symmetric stretching vibration of the U–F bond of Na₂UF₈ and it slightly red-shifted with the increase of the temperature (as shown in Table 1). At the same time, the peaks below 500 cm⁻¹ gradually widened apparently, which was because of the increase of the U–F bond length and the amplitude of the corresponding stretching vibration. In addition, a new weak band appeared around 818 cm⁻¹ when the temperature reached 300 °C as shown in Figure 1a. As the temperature continued to increase to about 320 °C, the intensity of characteristic vibrational frequency around 603 cm⁻¹ became very weak, and some new vibrational frequencies appeared at 278, 562, and 818 cm⁻¹, which implied that most of Na₂UF₈ were decomposed and some new compound formed on the NaF sorbent.

The vibrational frequency of Na₂UF₈ around 603 cm⁻¹ completely disappeared above 320 °C, and the vibrational frequencies of the new compound almost remain unchanged in the temperature range of 350–450 °C, which means that the Na₂UF₈ complex was unstable above 320 °C in the argon atmosphere by decomposition to NaF and UF₆. Moreover, the new compound might also transform from Na₂UF₈, and it was stable under 450 °C. As shown in Figure 1b, the blank NaF sorbent was tested as the reference under the same conditions, and no observable band was found in the Raman spectra from 25 to 450 °C.

To further determine the decomposition process of the Na₂UF₈ complex, the micromorphology of the Na₂UF₈ complex on the NaF sorbent before and after desorption at different temperatures was analyzed by scanning electron microscopy (SEM, Merlin compact, ZEISS, Germany). As shown in Figure 2, it was observed that the Na₂UF₈ complex coating on the surface of the NaF crystalline grain was a thick and compact layer (Figure 2a,b) at room temperature. The complex layer became thin and sparse due to the release of UF₆.

| temperature (°C) | 25 | 100 | 150 | 200 | 250 | 300 |
|-----------------|----|-----|-----|-----|-----|-----|
| wavenumber (cm⁻¹) | 609 | 608 | 607 | 606 | 604 | 603 |

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Figure 1. In situ Raman spectroscopy analysis of (a) Na₂UF₈ and (b) blank NaF.

Figure 2. Micromorphology of cross sections of the Na₂UF₈ complex before (a,b) and after desorption at 300 °C (c,d) and 350 °C (e,f).
when the temperature was 300 °C (Figure 2c,d). Compared to the blank NaF sorbent, the surface of NaF crystalline grains became rough and uneven at 350 °C (Figure 2e,f), and the Na2UF8 complex completely disappeared.

From the abovementioned results, it can be confirmed that Na2UF8 is relatively stable in the argon atmosphere below 300 °C; most Na2UF8 were decomposed into NaF and UF6 when the temperature was above 320 °C; meanwhile, a small amount of Na2UF8 might transform into a new compound.

**Chemical Morphological Analysis of the Uranium Residue on the NaF Sorbent.** In order to ascertain the chemical morphology of the corresponding compound formed when the temperature was above 300 °C, XRD characterization of Na2UF8 and the residues obtained after desorption at 300, 350, and 400 °C were carried out, respectively.

As shown in Figure 3a,b, the chemical morphology of the uranium residue on the NaF sorbent after desorption at 300 °C was still Na2UF8. The content of uranium on the NaF sorbent decreased from 474 mg U/g NaF (as shown in Table 2) to 433 mg U/g NaF after desorption at 300 °C for 1 h, which indicated that the desorption of UF6 from the NaF sorbent was slow when the temperature was below 300 °C, and only a small amount of Na2UF8 was decomposed into NaF and UF6, which was consistent with the results of Raman spectra analysis.

As shown in Figure 3c,d, a new compound, namely, Na3UF7 (or UF4·3NaF), formed when the desorption temperature was 350 and 400 °C, and it remained on the NaF sorbent stably; the characteristic vibrational frequencies at 278, 562, and 818 cm⁻¹ might attribute to this compound. The results of inductively coupled plasma atomic emission spectrometry (ICP-AES) analysis (as shown in Table 2) show that the content of the uranium residue on the NaF sorbent after desorption at 350 and 400 °C for 1 h was 44.6 and 35.8 mg U/g NaF, respectively, and on-line analysis of the infrared spectrometer manifested that the most of uranium desorbed from the NaF sorbent was in the form of UF6 (characteristic absorption peak at 625 cm⁻¹, as shown in Figure 4).12

To further determine the change of the valence state and the coordination structure, the Na2UF8 before and after desorption was characterized by XAFS based on Shanghai synchrotron radiation facility. The near-edge absorption peaks of U L3 in these samples are shown in Figure 5a. Quantitative information about the local structures could be extracted by fitting the EXAFS data. The fits are plotted in Figure 5b,c, and the fitting results are listed in Table 3.

It can be seen from Figure 5a that the near-edge absorption edges of U L3 of Na2UF8 and after desorption at 300 °C were almost identical, and the absorption edges of U L3 after desorption at 350 and 400 °C were also consistent. The absorption edge energy of U L3 of the uranium residue after desorption at 350 and 400 °C (the purple and the green lines) shifted about 2 eV to the low energy when they were compared to that of Na2UF8 before and after desorption at 300 °C (the black and the red lines), which indicated that the valence of uranium in the Na2UF8 complex was declined when the temperature exceeded 300 °C.13-16

The coordination environment of the U atom in Na2UF8 before and after desorption at 300 °C was significantly different from those after desorption at 350 and 400 °C. As shown in Figure 5b,c, in the R-range of 1-3.0 Å, the first two fitted well with Na2UF8 and the other two fitted well with NaUF. As shown in Table 3, the length of U-F bonds in Na2UF8 before and after desorption at 300 °C was 2.11 ± 0.01 and 2.12 ± 0.04 Å, respectively,17 the U-F bond lengths after desorption at 350 and 400 °C in the argon atmosphere were 2.18 ± 0.01 Å.18
The abovementioned results were consistent with the results of XRD analysis, and it further verified that the valence of uranium on the NaF sorbent was reduced from U (VI) to U (IV) after desorption. However, no evidence showed that U (V) existed in the decomposition process of Na2UF8 in our research, which may be due to the structural instability of the UF5−NaF complex. From the above experimental results, it can be concluded that the Na2UF8 complex was relatively stable in the range of 25−200 °C, and it began to decompose into NaF and UF6 at a low desorption rate in the range of 250−300 °C; the desorption rate increased quickly when the temperature was above 300 °C with most Na2UF8 decomposing into NaF and UF6, according to eq 1

\[
\text{Na}_2\text{UF}_8 \rightarrow 2\text{NaF} + \text{UF}_6 \uparrow
\]  

(1)

Meanwhile, a small amount of Na3UF7 was converted into Na3UF7 when the temperature was above 320 °C; according to eq 2, the Na3UF7 complex was very stable in the range of 350−450 °C under the argon atmosphere, which indicated that the desorption of UF6 from the NaF sorbent should be conducted under the fluorine atmosphere for the purpose of reducing the loss of uranium on the NaF sorbent and improving the utilization efficiency of the NaF sorbent.

\[
3\text{Na}_2\text{UF}_8 \rightarrow 2\text{Na}_3\text{UF}_7 + \text{UF}_6 \uparrow + \text{UF}_6 \uparrow
\]  

(2)

CONCLUSIONS
The present study demonstrated that the thermal stability of Na2UF8 complex and the formation mechanism of uranium residue during its decomposition under argon atmosphere. The results obtained from in situ Raman spectroscopy, SEM, XRD and XAFS analysis showed that the desorption of UF6 from Na2UF8 mainly went through the following stages in argon atmosphere, Na2UF8 was decomposed into NaF and UF6 rapidly when the temperature was over 320 °C, at the same time, a small amount of Na2UF8 complex was transformed to Na3UF7. The Na3UF7 remained on the NaF sorbent was stable in argon atmosphere even at 450 °C. The formation mechanism of Na3UF7 was presumed to be 3Na2UF8 → 2Na3UF7 + UF6↑ + 2F2↑. From the results of this research, it

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Table 2. Content of U on the NaF Sorbent after Desorption at Different Temperatures

| sample      | temperature (°C) | content of U (mg U/g NaF) |
|-------------|------------------|---------------------------|
| Na2UF8      | 25               | 474                       |
|             | 300              | 433                       |
|             | 350              | 44.6                      |
|             | 400              | 35.8                      |

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Figure 4. Infrared spectrum of outlet gas from the first absorber during desorption.

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Figure 5. (a) XANES spectra of U L3 edge, (b) FT of the U L3-edge EXAFS spectra of Na2UF8 and after desorption at 300 °C, and (c) after desorption at 350 and 400 °C.

Table 3. Structural Parameters from the EXAFS Spectra at the U L3 Edge of Na2UF8 before and after Desorption at 300, 350, and 400 °C in the Argon Atmosphere

| sample bond type | N  | R (Å) | \(\sigma \times 10^{-3} (\text{Å}^2)\) | R factor |
|------------------|----|-------|---------------------------------|----------|
| UF6=NaF (Na2UF8) | 8  | 2.11 ± 0.02 | 10 ± 1                          | 0.01     |
| 300 °C desorbed  | 8  | 2.12 ± 0.04 | 16 ± 2                          | 0.01     |
| 350 °C desorbed  | 7  | 2.18 ± 0.01 | 5.3 ± 0.5                       | 0.01     |
| 400 °C desorbed  | 7  | 2.18 ± 0.01 | 3.9 ± 0.4                       | 0.01     |
can be concluded that temperature does play an important role in the decomposition of Na₂UF₆ and to avoid the loss of the uranium and improve the reusability of the NaF sorbent, desorption of UF₆ from NaF sorbent should be carried out under fluorne atmosphere.

**EXPERIMENTAL SECTION**

**Reagents and Materials.** NaF sorbent (ϕ: 4 × 4 mm, specific surface area: 0.3–0.4 m²/g, porosity: 40–45%, strength: 6–8 kgf/cm²) was prepared in our laboratory.¹⁹ UF₄ was supplied by North Nuclear Fuel Co., Ltd.; Ar (99.999%) provided by Shanghai Xiangqun Special Gas Co., Ltd. was used as carrier gas in the adsorption and desorption experiments; F₂/He (20: 80 by volume, >99.99%) was provided by Beijing Hycegas Co., Ltd.

**Preparation of Na₂UF₆ Complex.** Na₂UF₆ complex was prepared on a home-made experiment setup as shown in Figure 6. The preparation process was as follows: a certain amount of NaF sorbent and UF₄ powder were placed in first adsorber and fluorinator, respectively; the F₂/He gas was used to pre-treat the fluorinator, pipeline and NaF sorbent to remove the possible moisture and avoid the hydrolysis of prepared UF₆. Then, the temperature of the first adsorber and the fluorinator was set to 100 and 380 °C, respectively; the UF₆ produced by the fluorination of UF₄ was adsorbed by NaF sorbent in the first adsorber, and Na₂UF₆ complex formed. The fluorination process was monitored by Fourier transform infrared (FTIR) spectroscopy (PerkinElmer Frontier; ZnSe as a reference: 4200–550 cm⁻¹; resolution: 4 cm⁻¹; scanning frequency: 32; optical path length: 10 cm). The second adsorber was mainly used to recover UF₆ penetrating from first adsorber. The adsorption capacity of NaF sorbent for UF₆ was determined by electronic balance. The prepared Na₂UF₆ complex was stored in a desiccator which was placed in the argon covered glovebox (oxygen content <1 ppm) for subsequent experiments.

**In Situ Analysis of the Na₂UF₆ Complex.** The in situ Raman spectra of the Na₂UF₆ complex from 25 to 450 °C in the argon atmosphere were recorded using a HORIBA Jobin Yvon LabRAM HR800 Raman spectrometer which was equipped with a Linkam TS1000 microscopic heating furnace with a temperature accuracy of ±1 °C. The test process was as follows: first, the Na₂UF₆ complex sample was added into a Pt crucible, which was placed in the furnace and sealed in the argon covered glovebox; then, the furnace was connected to the Raman spectrometer and heated to the setting temperature at a rate of 10 °C/min, with introduction of pure argon at a flow rate of 20 mL/min. The blank NaF sorbent was also tested as reference under the same conditions.

**Preparation of the Uranium Residue on the NaF Sorbent.** In order to determine the chemical morphology of the uranium residue on the NaF sorbent after desorption in the argon atmosphere, the desorption experiments of the Na₂UF₆ complex were carried out on the same experimental setup used in preparation of the Na₂UF₆ complex. First, the prepared Na₂UF₆ complex was loaded in the first adsorber, and pure argon gas with a flow rate of 20 mL/min was inlet as carrier gas. Then, both adsorbers and the pipeline were heated to 100 °C. After the temperature reached 100 °C, the first adsorber was heated to the specified temperature for desorption with the desorption process being monitored by FTIR. The content of the uranium on the NaF sorbent after desorption was measured by ICP-AES (Optima 8000, PerkinElmer, USA).

**Morphological Analysis of the Uranium Residue on the NaF Sorbent.** The chemical morphology of uranium on the NaF sorbent before and after desorption at different temperatures was characterized by standard powder X-ray diffraction with CuKα radiation (XRD, PANalytical X′Pert Pro MPD X-ray polycrystalline diffractometer, DY3614, Netherlands) and XAFS. All of the samples were prepared in an argon glovebox. The sample was wrapped with the polymer film to prevent the contact with water and oxygen during the analysis process. The diffraction patterns were obtained over a 2θ range of 10°–90° with a scanning step size of 0.01°.

The XAFS analysis process was as follows: first, the sample was ground, pressed, and sealed (to prevent the sample from contacting with water and oxygen in the atmosphere during the analysis process) in the glovebox; second, the XAFS analyses were carried out at Shanghai Synchrotron Radiation Facility (SSRF) and BL14W1 beam experimental station²⁰ with a Si(311) double crystal monochromator in the nonfocusing mode for U L₃-edge. The electron beam energy of the storage ring was 3.5 GeV, and the maximum storage current was about 250 mA. The L₃-edge EXAFS data of U were analyzed by the standard procedures in Demeter.²¹ The theoretical phase and amplitude functions were calculated with the program FEFF 9.0.²² Finally, the fitting procedure was performed on the k²-weighted FT-EXAFS data from 2.2 to 11.5 Å⁻¹. An R window of 1–3 Å was used for the fitting. The amplitude reduction factor S₀ was fixed at 1 in the EXAFS fits, and the shifts in the threshold energy ∆E₀ were constrained to be the same value for all fitted shells. The coordination numbers (N), interatomic

Figure 6. Flow diagram of the experimental setup.
distances \((r)\), and Debye–Waller factors \((\Delta\sigma^2)\) were left as free parameters.

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