Supplementary Information (SI) for Green Chemistry.
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Supplementary Information

A green route for producing high-purity nano-SiO_2 from silicon containing waste

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Supplementary Materials 1（S1）：

(1) Acid Leaching Pretreatment of Silica Fume

Silica fume (50 g) was treated with 300 mL of hydrochloric acid. The acid leaching was carried out at 40 ℃ for 60 minutes with a stirring rate of 300 rpm. The effect of HCl concentration on the SiO_2 content in silica fume is shown in Figure 1(a). As seen in Figure 1(a), the SiO_2 content in silica fume increases rapidly with increasing HCl concentration, and then the growth rate gradually slows down. When the HCl concentration exceeds 2 mol/L, the leaching rate of metal oxides tends to slightly decrease with further increase in acid concentration. This is because a higher acid concentration intensifies the salting-out effect in the reaction system, leading to a lower apparent leaching rate in the measurements. Therefore, an HCl concentration of around 2 mol/L is considered optimal.

Silica fume: 50 g; HCl volume: 300 mL; acid leaching temperature: 40 ℃; HCl concentration: 2 mol/L; stirring rate: 300 rpm. The effect of reaction time on the SiO_2 purity in silica fume is shown in Figure 1(b). As depicted, the SiO_2 content increases rapidly with reaction time between 30-120 minutes. However, when the reaction time exceeds 120 minutes, the increase in SiO_2 content becomes more gradual. This indicates that metal oxides in the silica fume cannot be fully leached in a short time, and the reaction gradually approaches equilibrium with prolonged duration. Beyond 120 minutes, the leaching rate of metal oxides remains relatively constant. Therefore, a reaction time of approximately 120 minutes is deemed suitable.

Silica fume: 50 g; HCl volume: 300 mL; HCl concentration: 2 mol/L; leaching time: 120 min; stirring rate: 300 rpm. As shown in Figure 1(c), increasing the reaction temperature leads to a higher SiO_2 purity. At 60 ℃ and 70 ℃, the SiO_2 content is comparable. Further increasing the reaction temperature does not significantly improve the purity of SiO_2. This is attributed to the rapid volatilization of HCl at high temperatures, which generates acid mist in the air. Based on these findings, a reaction temperature of 60 ℃ is considered appropriate.

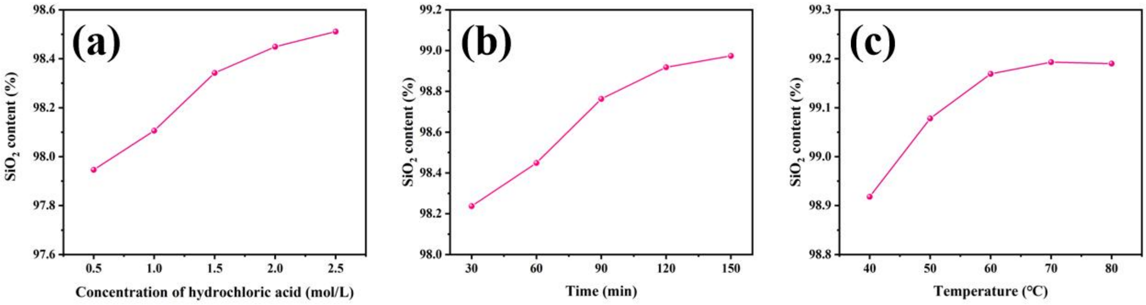

Fig.1(a) Effect of acid concentration on SiO_2 content, (b) Effect of reaction time on SiO_2 content, (c) Effect of reaction temperature on SiO_2 content

(2) Alkaline Dissolution of Silica Fume for Sodium Silicate Preparation

Under the conditions of a reaction temperature of 90 °C, a liquid-to-solid ratio of 6:1, and a reaction time of 2 hours, the effect of sodium hydroxide concentration on the leaching rate of SiO_2 was investigated. The results are shown in Figure 2(a). As seen in Figure 2(a), a low NaOH concentration results in poor SiO_2 extraction. However, with increasing NaOH concentration, the SiO_2 extraction efficiency improves significantly. When the NaOH concentration increases from 5% to 20%, the leaching rate of SiO_2 improves markedly. Once the concentration exceeds 20%, the reaction system becomes more viscous, leading to gel formation on the inner wall and bottom of the reactor. This reduces the flowability of the reactants, impedes diffusion, and ultimately slows down the reaction rate, thereby decreasing the leaching efficiency of SiO_2.

At a NaOH concentration of 20%, reaction temperature of 90 °C, and reaction time of 2 hours, the effect of the liquid-to-solid ratio on the leaching rate of SiO_2 was studied. The results are shown in Figure 2(b). As seen in Figure 2(b), when the liquid-to-solid ratio is below 6:1, increasing the ratio significantly enhances the extraction efficiency of SiO_2. However, when the ratio exceeds 6:1, the improvement rate slows down. At a constant NaOH concentration, a moderate liquid-to-solid ratio can effectively reduce alkali consumption and lower production costs. A too-low ratio results in a slurry that is too thick, negatively impacting mass transfer and lowering the leaching rate. Increasing the liquid-to-solid ratio improves slurry flowability, accelerates mass transfer and reaction rates. Therefore, a liquid-to-solid ratio of 6:1 is selected.

At a NaOH concentration of 20%, liquid-to-solid ratio of 6:1, and reaction time of 2 hours, the effect of reaction temperature on the leaching rate of SiO_2 was studied. The results are shown in Figure 2(c). As observed, reaction temperature has a significant effect on the leaching rate. The leaching rate of SiO_2 increases rapidly with rising temperature. In a solid-liquid reaction system, elevated temperature enhances the thermal motion of molecules and promotes the transition of non-activated molecules into activated ones, resulting in more molecules participating in the reaction and accelerating the reaction rate. Therefore, raising the leaching temperature improves the leaching rate of SiO_2 from silica fume. The reaction reaches optimal efficiency at 90 °C. Further increasing the temperature leads to only a slight increase in leaching rate. Considering both economic benefits and leaching efficiency, 90 °C is considered the most suitable reaction temperature.

At a NaOH concentration of 20%, liquid-to-solid ratio of 6:1, and reaction temperature of 90 °C, the effect of reaction time on the leaching rate of SiO_2 was investigated. The results are shown in Figure 2(d). As shown, the leaching rate increases with prolonged reaction time. Before 2 hours, the leaching rate increases rapidly, and after that, the increase becomes gradual. As the reaction time extends, NaOH and silica fume have sufficient mixing and contact in the solution, leading to a more complete reaction. Once dynamic equilibrium is reached, further extension of the reaction time has little effect on the leaching rate of SiO_2 and may even cause gelation of the sodium silicate solution, which is unfavorable for subsequent reactions. Therefore, the reaction time should be controlled within 2.5 hours.

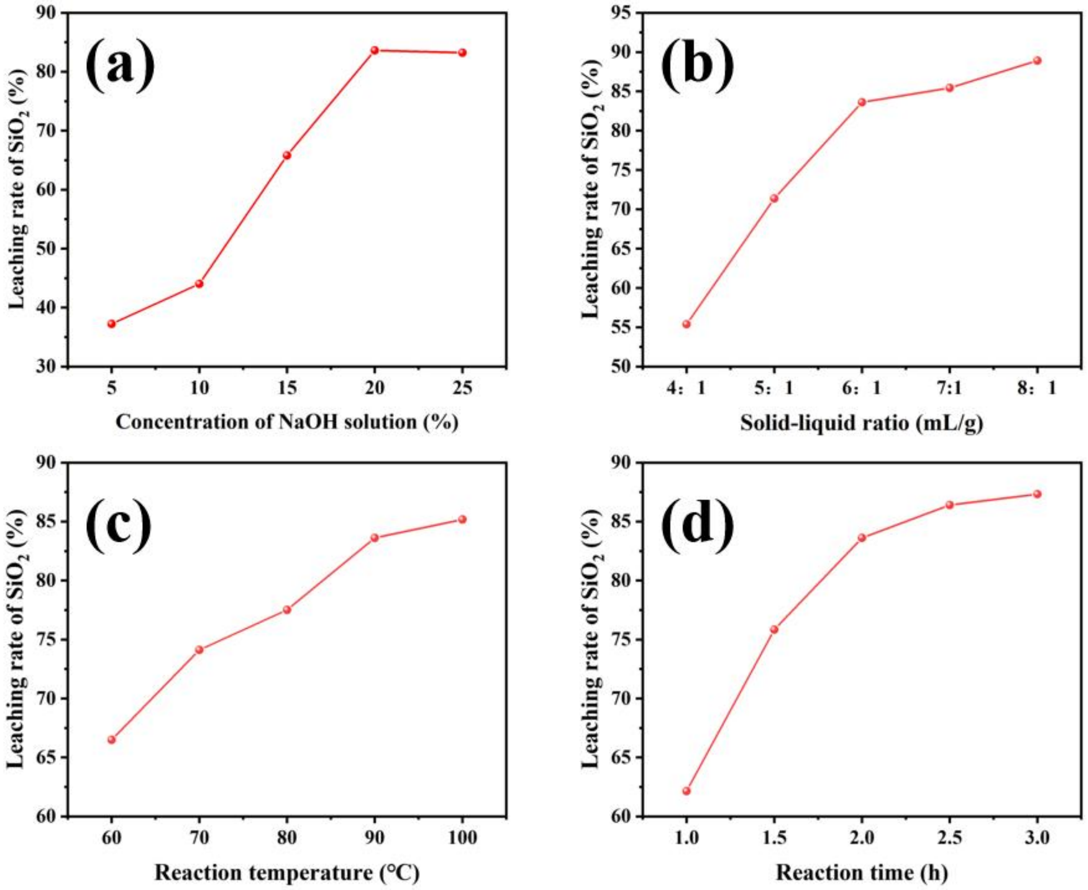

Fig.2 (a) Effect of sodium hydroxide mass fraction on the leaching rate of SiO_2, (b) Effect of reaction time on the leaching rate of SiO_2, (c) Effect of reaction temperature on the leaching rate of SiO_2, (d) Effect of reaction time on the leaching rate of SiO_2

Supplementary Materials 2（S2）：

The following pictures are additional scanning electron microscope (SEM) images of SiO_2 at different magnifications, used to more clearly observe the micro-morphology of the prepared SiO_2.

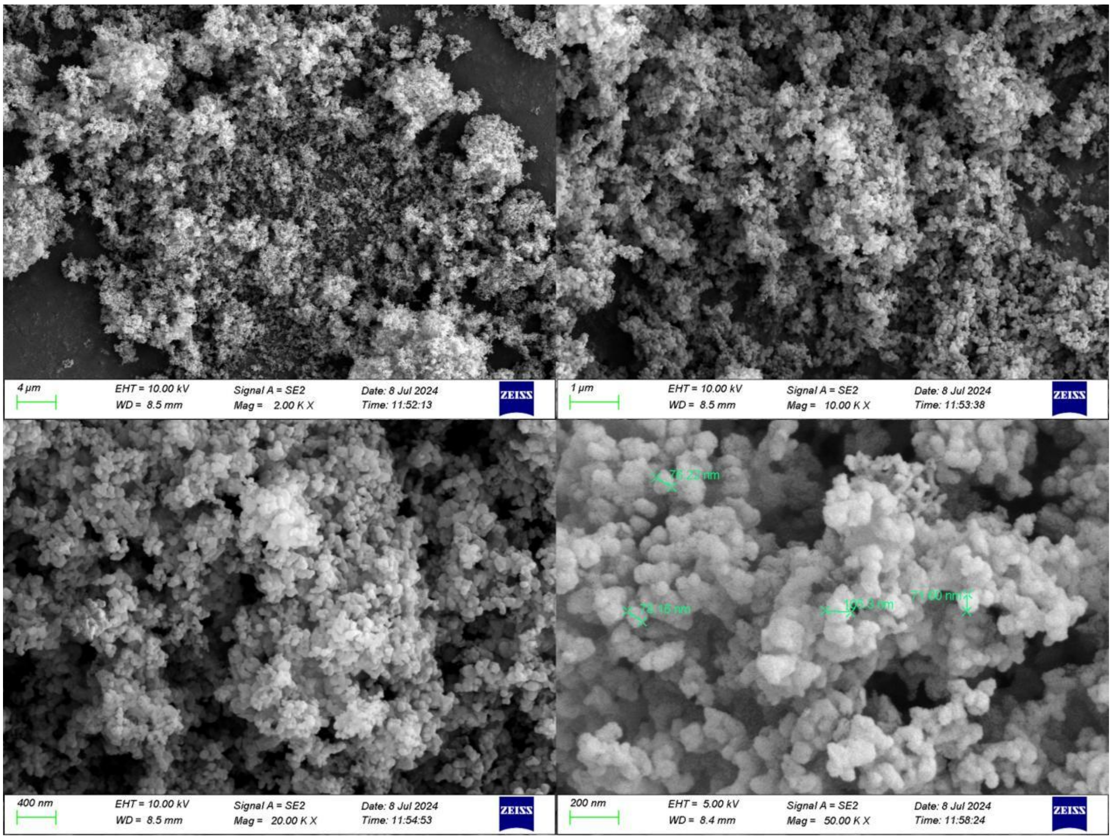

Fig.3 SEM Images at Different Magnifications

Supplementary Materials 3（S3）：

Further Purification of Silicon Dioxide

First, 100 mL of EDTA-2Na solution at the required concentration was prepared and measured. Then, 5 g of crude SiO_2 powder obtained from previous experiments was accurately weighed as the raw material. The SiO_2 powder and the EDTA-2Na solution were added into a 200 mL conical flask and mixed thoroughly. During the experiment, the pH of the system was adjusted using sulfuric acid and ammonia solution. The conical flask was then placed on a thermostatic magnetic stirring device to carry out the chelating impurity removal experiment. EDTA-2Na, serving as the chelating agent, could coordinate with metal impurity ions adsorbed on the surface of spherical SiO_2 particles, promoting the formation of water-soluble coordination compounds, thereby achieving the goal of impurity leaching.

Subsequently, mixed acid leaching was investigated. A 5 g sample of SiO_2 after chelating treatment was used to study the effect of hydrochloric acid concentration on impurity removal, under the conditions of a liquid-to-solid ratio of 6:1, reaction temperature of 80 ℃, and leaching time of 120 min. After determining the optimal concentration of hydrochloric acid, oxalic acid was added to the system to evaluate the effect of its concentration. Based on the optimal concentrations of hydrochloric acid and oxalic acid, citric acid was further introduced, and its effect on impurity removal was discussed. After determining the optimal composition and concentrations of the mixed acids, the influence of liquid-to-solid ratio, leaching temperature, and leaching time on impurity removal efficiency was investigated. After leaching, the product was washed and dried. The process flow for further purification of SiO_2 is illustrated in Figure 4.

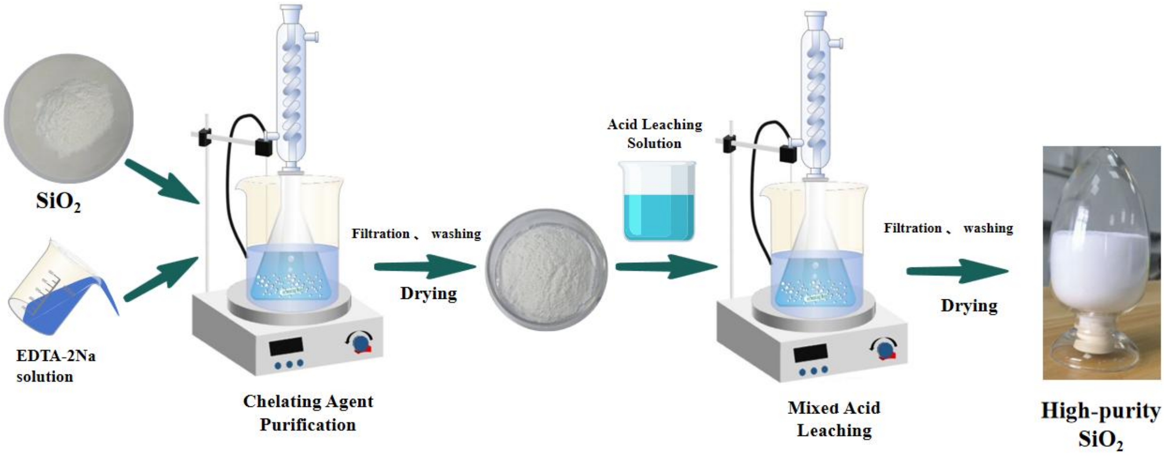

Fig. 4. Schematic diagram of impurity removal by chelating agents and mixed acid leaching for the preparation of high-purity SiO_2

(1) Impurity Removal by Chelating Agent

Under the experimental conditions of solution pH = 3, reaction temperature 50 °C, and reaction time 120 min, the effect of EDTA-2Na concentration on the impurity content in SiO_2 and the corresponding removal efficiency is shown in Figure 5(a). As can be seen, the contents of Al, Ca, and Fe impurities in the crude SiO_2 decreased with increasing EDTA-2Na concentration. Among them, the removal of Al was the most significant. As shown in Figure 5(a), when the EDTA-2Na concentration increased from 0.01 mol/L to 0.1 mol/L, the removal efficiencies of Al, Ca, and Fe increased gradually. This can be attributed to the increased concentration of the chelating agent, which effectively enhances the reaction driving force by increasing the concentration of reactants. At an EDTA-2Na concentration of 0.1 mol/L, the removal efficiencies of Al, Ca, and Fe reached 64.26%, 66.58%, and 39.93%, respectively. However, when the concentration exceeded 0.1 mol/L, further increases had little effect on the removal efficiencies. This may be due to the limited solubility of the impurities in SiO_2, meaning that even an excess of EDTA-2Na could not further dissolve the remaining poorly soluble impurities. At the same concentration, EDTA-2Na exhibited better removal efficiency for Al and Ca compared to Fe.

Under the conditions of EDTA-2Na concentration 0.1 mol/L, reaction temperature 50 °C, and reaction time 120 min, the influence of solution pH on impurity content and removal efficiency is shown in Figure 5(b). The data indicate that the Al content in the SiO_2 powder showed the most significant variation. When EDTA-2Na was used as the chelating agent to remove Al impurities from the surface of SiO_2 particles, solution pH had a pronounced effect on the chelating performance. Specifically, pH affects both the binding capacity of EDTA with metal ions and the solubility of metal ions. At lower pH values, the chelating ability of EDTA is relatively weak because the carboxyl groups (-COOH) of EDTA remain mostly in their undissociated form under acidic conditions, limiting their ability to form stable chelates with metal ions. Moreover, Al has low solubility in acidic conditions, which inhibits its dissolution from the SiO_2 surface into the solution, thereby reducing removal efficiency. When the solution pH was adjusted to 5, the carboxyl groups of EDTA partially dissociated to $–COO^-$, enabling effective chelation with metal ions and thus achieving higher removal efficiency. pH variation had little effect on Ca, whereas it had a negative effect on Fe removal: as pH increased from 2 to 7, the Fe content in SiO_2 rose from 90.34 μg/g to 106.46 μg/g, and the Fe removal efficiency decreased from 45.23% to 35.45%. Considering the overall removal performance for all impurities, a solution pH of 5 was selected.

Under the conditions of EDTA-2Na concentration 0.1 mol/L, solution pH = 5, and reaction time 120 min, the effect of reaction temperature on impurity content and removal efficiency is shown in Figure 5(c). The figure shows that the removal efficiencies of Al, Ca, and Fe followed similar trends with increasing temperature.

The temperature had a relatively small effect on the chelating removal efficiency. However, the reduction in Al content was more pronounced compared to Ca and Fe. When the temperature increased from 30 °C to 50 °C, the Al content decreased from 266.68 μg/g to 227.62 μg/g. In contrast, the changes in Ca and Fe contents were less significant, decreasing from 55.48 μg/g and 106.29 μg/g to 50.91 μg/g and 98.31 μg/g, respectively. Therefore, the reaction temperature was set at 50 °C.

Under the conditions of EDTA-2Na concentration 0.1 mol/L, solution pH = 5, and reaction temperature 50 °C, the influence of reaction time on impurity content and removal efficiency is shown in Figure 5(d). The data indicate that from 30 min to 90 min, the removal efficiency of impurities increased rapidly with time. After 90 min, the removal efficiencies of Al and Ca gradually stabilized, while the Fe removal efficiency showed some fluctuation. This may be due to the fast chelation reaction between impurity ions and EDTA-2Na, which approached equilibrium within 90 min. Therefore, when using EDTA-2Na to remove Al, Ca, and Fe from crude SiO_2, a reaction time of 90 min is sufficient to meet the purification requirements. At this point, the removal efficiencies of Al, Ca, and Fe reached 66.75%, 67.65%, and 43.47%, respectively, and their residual contents in SiO_2 were 218.74 μg/g, 51.19 μg/g, and 93.24 μg/g. Extending the reaction time further would not significantly improve impurity removal and would reduce experimental efficiency. Hence, a reaction time of 90 min was selected.

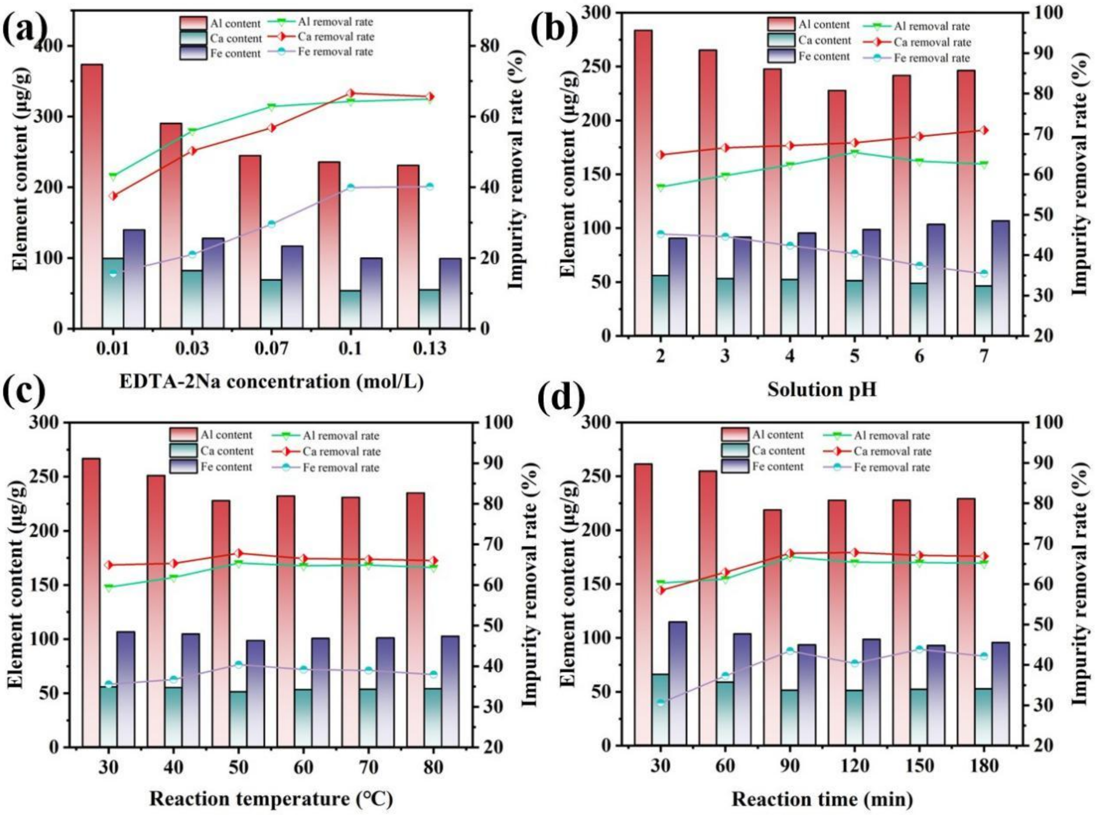

Fig. 5. Effects of process parameters on impurity content and removal rate of SiO_2: (a) EDTA-2Na concentration, (b) Solution pH, (c) Reaction temperature, (d) Reaction time

(2) Impurity Removal via Mixed Acid Leaching

The concentration of hydrochloric acid (HCl) was set to 1, 2, 3, 4, and 5 mol/L, respectively. A fixed liquid-to-solid ratio of 6:1 (mL/g) was maintained, and the acid solutions were added to Erlenmeyer flasks containing SiO_2. The mixtures were magnetically stirred at 80 °C for 120 minutes. The effects of HCl concentration on the content and removal rates of Al, Ca, and Fe in SiO_2 are shown in Fig. 6(a). The results demonstrate that HCl concentration has a significant influence on the removal efficiency of metallic impurities. As the acid concentration increased, the removal rates of all impurities showed an upward trend. The overall removal rate exhibited two distinct stages. When the HCl concentration ranged from 1 to 4 mol/L, higher acid concentrations provided more abundant leaching species and accelerated the leaching reactions, thereby increasing the removal rates of Al, Ca, and Fe. During this stage, the removal curves had a steep slope, indicating vigorous reactions. Increasing the concentration of the acidic medium further promoted the forward progression of the reaction and activated more reactive molecules, thus enhancing the efficiency of impurity removal. However, when the HCl concentration increased from 4 to 5 mol/L, the slope of the removal curves flattened, suggesting a deceleration in the reaction rate. This could be attributed to the formation of a dense product layer within a short time at excessively high acid concentrations, which may hinder the reaction process and gradually reduce the improvement in removal efficiency. When the HCl concentration reached 4 mol/L, the removal rates of Al, Ca, and Fe were 57.13%, 31.08%, and 36.53%, respectively. Further increasing the HCl concentration to 5 mol/L resulted in only minor improvements in removal rates. Considering that lower acid concentrations are preferred in industrial applications, an HCl concentration of 4 mol/L was selected for subsequent experiments.

Under the condition of 4 mol/L HCl, oxalic acid was added at concentrations of 0.05, 0.08, 0.11, 0.14, and 0.17 mol/L, respectively. The same liquid-to-solid ratio of 6:1 (mL/g) was used, and the mixtures were magnetically stirred at 80 °C for 120 minutes. The effects of oxalic acid concentration on the content and removal rates of Al, Ca, and Fe in SiO_2 are shown in Fig. 6(b). Oxalic acid is generally considered a more environmentally friendly and effective reagent for leaching Fe impurities in industrial-grade quartz. As shown in Fig. 6(b), the increase in oxalic acid concentration had the most pronounced effect on Fe content and removal rate. This can be attributed to the reaction between oxalic acid and Fe; thus, higher oxalic acid concentrations should favor Fe removal. However, when the oxalic acid concentration exceeded a certain threshold, further increases did not lead to higher Fe removal rates, resulting in a plateau effect. When the oxalic acid concentration was below 0.11 mol/L, hydrolysis occurred, producing large amounts of $HC_2O_4^-$ and $C_2O_4^{2-}$, which readily complexed with Fe_2O_3 and other impurities, significantly enhancing impurity removal. In contrast, increasing the oxalic acid concentration from 0.11 to 0.17 mol/L suppressed its hydrolysis due to excess addition, thereby reducing the availability of $HC_2O_4^-$ and $C_2O_4^{2-}$ in the solution and ultimately diminishing impurity removal efficiency. Therefore, 0.11 mol/L was determined to be the optimal concentration of oxalic acid.

Based on a mixed acid system containing 4 mol/L HCl and 0.11 mol/L oxalic acid, citric acid was further added at concentrations of 0.01, 0.03, 0.05, 0.07, and 0.09 mol/L. With the same liquid-to-solid ratio of 6:1 (mL/g), the mixtures were magnetically stirred at 80 °C for 120 minutes. The effects of citric acid concentration on the content and removal rates of Al, Ca, and Fe in $[C_6H_5O_7]^{3-}$ are shown in Fig. 6(c). Citric acid, as a leaching agent, exhibits strong reactivity toward metal oxides and has negligible corrosiveness to reaction vessels made of stainless steel, making it more suitable for industrial applications. The hydroxyl and carboxyl functional groups in citric acid molecules can coordinate with metal ions at multiple sites to form stable, liquid-phase, multi-ring metal complexes, thereby enabling effective removal of metal impurities from SiO_2. As shown in Fig. 6(c), increasing the concentration of citric acid improved impurity removal. A higher concentration of citric acid corresponded to higher removal rates. When the citric acid concentration increased from 0.01 mol/L to 0.07 mol/L, citric acid ions ($[C_6H_5O_7]^{3-}$) promoted the complexation reactions with impurity ions, enhancing their removal. However, when the citric acid concentration exceeded 0.07 mol/L, the excessive presence of citrate ions inhibited subsequent hydrolysis reactions, thereby reducing impurity removal efficiency or slowing the rate of increase.

Using 4 mol/L hydrochloric acid, 0.11 mol/L oxalic acid, and 0.07 mol/L citric acid as the optimal acid leaching combination, mixed acid solutions with liquid-to-solid ratios of 4:1, 6:1, 8:1, 10:1, and 12:1 (mL/g) were added to conical flasks containing SiO_2. The mixtures were stirred magnetically at 80 ℃ for 120 minutes to investigate the effect of liquid-to-solid ratio on the content and removal efficiency of Al, Ca, and Fe in SiO_2, as shown in Figure 6(d). When the liquid-to-solid ratio was 4:1, the removal efficiency of impurities was the lowest. This may be attributed to the relatively loose structure of the prepared SiO_2 powder, where insufficient acid volume leads to high solution viscosity, resulting in incomplete leaching. In addition, a smaller liquid-to-solid ratio may cause the slurry to adhere to the walls of the container under magnetic stirring, leading to uneven acid leaching and poor purification performance. As the liquid-to-solid ratio increased, the viscosity of the slurry decreased, and the diffusion rate increased. This enhanced the contact between SiO_2 particles and H^+ ions during leaching, facilitating the diffusion of H^+ into the interior of the particles and improving the removal efficiency of impurities. However, an excessively high liquid-to-solid ratio requires more acid solution, increasing purification costs and generating more waste acid. When the liquid-to-solid ratio increased from 8:1 to 10:1, the removal efficiencies of Al, Ca, and Fe only increased slightly from 79.09%, 72.98%, and 77.83% to 81.14%, 74.39%, and 80.62%, respectively. Therefore, from an economic perspective, a liquid-to-solid ratio of 8:1 is a more appropriate choice.

Using the same optimal acid combination and a liquid-to-solid ratio of 8:1 (mL/g), acid leaching was carried out in beakers containing SiO_2 at different temperatures (50, 60, 70, 80, and 90 °C) with magnetic stirring for 120 minutes. The effect of temperature on the content and removal efficiency of Al, Ca, and Fe in SiO_2 was investigated, as shown in Figure 6(e). As illustrated, increasing the leaching temperature significantly improved the impurity removal efficiency. With rising temperature, the removal rates of Al, Ca, and Fe increased substantially. This is because higher temperatures accelerate chemical reaction rates. As the reaction temperature increases, molecular kinetic energy rises, enabling a greater fraction of low-energy molecules to be activated. The proportion of activated molecules in the system thereby increases. At the same time, intensified molecular motion enhances collision frequency, increasing the number of effective collisions per unit time, thereby accelerating the reaction rate and significantly improving the leaching of Al, Ca, and Fe. At 80 °C, the leaching rates of Al, Ca, and Fe reached 79.09%, 72.98%, and 77.83%, respectively. Although further improvements were observed at 90 °C, the increase was marginal. This may be due to the increased evaporation of HCl at higher temperatures, which lowers the actual acid concentration and reduces the impurity dissolution efficiency. Therefore, 80 °C is considered a reasonable leaching temperature.

Using the optimal acid combination and a liquid-to-solid ratio of 8:1 (mL/g), acid leaching was conducted in conical flasks containing SiO_2 at 80 °C with magnetic stirring for varying durations (60, 90, 120, 150, 180, and 210 minutes) to investigate the effect of reaction time on the content and removal efficiency of Al, Ca, and Fe in SiO_2, as shown in Figure 6(f). The results showed that the removal efficiencies of Al, Ca, and Fe increased gradually with prolonged reaction time, with the removal of Ca being most affected by the duration. When the reaction time reached 180 minutes, the leaching rates of Al, Ca, and Fe were 86.61%, 93.55%, and 92.88%, respectively. Further extending the reaction time to 210 minutes resulted in leaching rates of 86.85%, 93.92%, and 92.27%, respectively. These results indicate that the increase in removal efficiency slowed and tended to stabilize after 3 hours, suggesting that reaction time significantly influences the extent of the leaching process. In general, prolonging the reaction time promotes a more complete reaction and improves impurity removal. However, excessively long durations may reduce production efficiency. Therefore, considering both purification performance and production efficiency, 180 minutes is selected as the optimal leaching time for the mixed acid system.

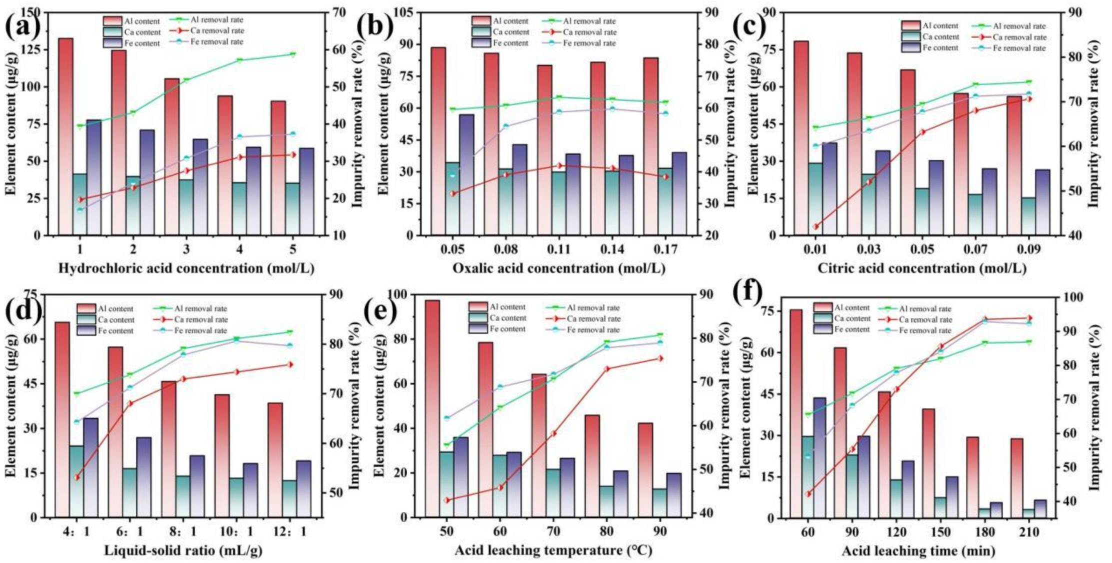

Figure 5 Effects of acid leaching conditions on impurity content and removal rate of SiO_2: (a) hydrochloric acid concentration, (b) oxalic acid concentration, (c) citric acid concentration, (d) liquid-to-solid ratio, (e) acid leaching temperature, (f) acid leaching time

Supplementary Materials 4（S4）：

Techno-economic feasibility analysis

1.Acid leaching pretreatment process of silica fume

Acid leaching conditions：HCl concentration 2mol/L、liquid-to-solid ratio 6：1. 1t the silica fume needs to be cleaned with 6,000 L of a 2 mol/L hydrochloric acid solution. Calculate the amount of HCl required:

$$n_{HCl} = c \times V = 2mol/L \times 6000L = 12000mol$$

Calculate the volume of concentrated hydrochloric acid needed (assuming the concentration of commercially available concentrated hydrochloric acid is 12 mol/L).：

$$V = \frac{12000mol}{12mol/L} = 1000L$$

2.Process of preparing sodium silicate by alkaline dissolution

In the alkaline dissolution process, 20% sodium hydroxide is used, and the liquid-solid ratio is 6:1 for dissolving silica fume. The mass change after acid leaching treatment is relatively small and can be neglected. Therefore, for 1 ton of silica fume, 6,000 L of 20% sodium hydroxide is consumed, and the mass of sodium hydroxide is 1.2 tons. The leaching rate of silica is 86.4%, so the mass of silica that reacts in the silica fume is:

M_{SiO2}=$M_{silica\ fume}$×97.68%×86.4%=0.8440t

The molar mass of SiO_2: 60.08 g/mol; The molar mass of NaOH: 40 g/mol; The molar mass of Na_2SiO_3: 122.06 g/mol.

Convert 0.8440 tons of silicon dioxide into moles:

$$n_{SiO2}=\frac{844000}{60.08}=14047.9\text{mol}$$

$$SiO_2+2NaOH\rightarrow Na_2SiO_3+H_2O\ （1）$$

For every 1 mole of SiO_2, 1 mole of Na_2SiO_3 is generated.

Calculate the mass of Na_2SiO_3 produced according to Equation (1):

$$\frac{122.06}{60.08}\times0.8440=1.7147\text{t}$$

That is, 1 ton of silica fume reacts with 1.2 tons of NaOH to produce 1.7147 tons of Na_2SiO_3.

3.Impurity removal from sodium silicate solution using calcium oxide

In the experiment, a sodium silicate solution with a silica concentration of 70 g/L was treated using calcium oxide at a concentration of 6 g/L.

The mass of silica in 1.7147 tons of Na_2SiO_3 is calculated as:

1.7147t×60.08/122.06=844000g。

Therefore, 1.7147 t of Na_2SiO_3 can be used to prepare 12,057.14 L of sodium silicate solution with a silica concentration of 70 g/L.

The required mass of calcium oxide is:

6g/L×12057.14L=72342.84g=0.07234t

During the calcium oxide impurity removal process, part of the silica in the solution is consumed. Under the optimal conditions for calcium oxide, 13.4% of the silica is lost. Therefore, the remaining mass of silica after impurity removal is:

844000g×（1-13.4%）=730904g。

4. Preparation of SiO_2 by carbonization method

Given that the silica recovery rate in the experiment is 92.4%, the mass of silica participating in Reaction (2) is calculated as:

730904g×92.4%=675355.3g

$$Na_2SiO_3+CO_2+H_2O\rightarrow SiO_2+Na_2CO_3(2)$$

Namely, 1 mol Na_2SiO_3 + 1 mol CO_2 → 1 mol SiO_2 + 1 mol Na_2CO_3. From this, the amount of carbon dioxide gas consumed can be calculated. (Molar mass of CO_2:

44.01 g/mol)

$$\frac{675355.3}{60.08} \times 44.01 = 494713.5\text{g} = 0.4947\text{t}$$

The volume at standard temperature and pressure (STP) is: (Under STP, the molar volume of a gas is approximately 22.4 L/mol.)

$$\frac{675355.3}{60.08} \times 22.4 = 251796.9\text{L}$$

The mass of Na_2CO_3 produced is (molar mass of Na_2CO_3: 106 g/mol):

$$\frac{675355.3}{60.08} \times 106 = 1191539\text{g}$$

5.Reaction of Na_2CO_3 with CaO to recycle $CaCO_3$

$$Na_2CO_3 + CaO + H_2O \to 2NaOH + CaCO_3 \quad （3）$$

The molar mass of Na_2CO_3 is 106 g/mol; the molar mass of CaO is 56.08 g/mol; the molar mass of $CaCO_3$ is 100.09 g/mol; the molar mass of NaOH is 40 g/mol.

Calculate the mass of CaO consumed in Reaction (3):

$$\frac{1191539}{106} \times 56.08 = 630391.6\text{g} = 0.6304\text{t}$$

Calculate the mass of $CaCO_3$ produced in reaction (3):

$$\frac{1191539}{106} \times 100.09 = 1125105\text{g} = 1.1251\text{t}$$

Namely, 1.1251 tons of $CaCO_3$ is produced.

The mass of NaOH produced is:

$$\frac{1191539}{106} \times 2 \times 40 = 899274.7\text{g} = 0.8993\text{t}$$

The 0.8993 tons of NaOH generated here can be used in the alkaline dissolution stage of silica fume. Thus, the mass of NaOH that needs to be consumed in the process is:

1.2t-0.8993t=0.3007t

6.Chelating agent impurity removal stage

During this stage, SiO_2 reacts with 0.1 mol/L EDTA-2Na at a liquid-to-solid ratio of 20:1, which requires:

675355.3g×20mL=13507106mL=13507.106L

The number of moles of EDTA-2Na consumed:

$$n = c \times V = 0.1\text{mol/L} \times 13507.106\text{L} = 1350.7106\text{mol}$$

The chemical formula of EDTA-2Na is $C_{10}H_{14}N_2Na_2O_8 \cdot 2H_2O$ (dihydrate, the common form).

Calculate the mass of EDTA-2Na required：

$$m = n \times M = 1350.7106\text{mol} \times 372.24\text{g/mol} = 502788.5\text{g} = 0.5028\text{t}$$

7. Mixed Acid Leaching Stage

A mixed acid solution composed of 4 mol/L hydrochloric acid, 0.11 mol/L oxalic acid, and 0.07 mol/L citric acid was used as the optimal leaching combination. The reaction was carried out at a liquid-to-solid ratio of 8:1 (mL/g) for impurity removal. A total of 675,355.3 g of silica was reacted with 5,402.8 L of the mixed acid solution.

Calculate the mass of EDTA-2Na required:

$$n = c \times V = 4\mathrm{mol/L} \times 5402.8\mathrm{L} = 21611.2\mathrm{mol}$$

Moles of hydrochloric acid required:

$$V = \frac{21611.2\mathrm{mol}}{12\mathrm{mol/L}} = 1800.9\mathrm{L}$$

The total amount of hydrochloric acid consumed is:

1000L+1800.9L=2800.9L=3.305t

Calculate the amount of oxalic acid ($H_2C_2O_4 \cdot 2H_2O$, molar mass: 90.03 g/mol) required:

$$m = 0.11\mathrm{mol/L} \times 5402.8\mathrm{L} \times 90.03\mathrm{g/mol} = 53505.5\mathrm{g} = 0.0535\mathrm{t}$$

Calculate the amount of citric acid (molar mass: 192.12 g/mol) required:

$$m = 0.07\mathrm{mol/L} \times 5402.8\mathrm{L} \times 192.12\mathrm{g/mol} = 72659\mathrm{g} = 0.07266\mathrm{t}$$

Table 1. Material costs and product value in the production process of high-purity silica from silica fume

	Name	Quantity (t)	Unit Price (CNY/ton)	Amount (CNY)
Raw Material Input	silica fume	1t	750	750
	hydrochloric acid	3.305	400	1322
	Sodium hydroxide	1.2t	2500	3000
	calcium oxide	0.70274t	500	351.37
	carbon dioxide	0.4947	650	321.56
	EDTA-2Na	0.5028t	9200	4625.76
	Oxalic acid	0.0535t	3200	171.2
	Citric Acid	0.07266t	4800	348.77
	total cost			10890.66
Product Output	Calcium carbonate	1.1251t	850	956.34
	Sodium hydroxide	0.8993t	2500	2248.25
	SiO_2（4N）	0.6754	30000	20262

Total Value	23466.59

According to the table, the material cost for processing one ton of silica fume using this process is 10,890.66 CNY. The total value of the output products reaches 23,466.59 CNY, with high-purity 4N-grade silicon dioxide contributing the most due to its high market price. Considering only the input and output of materials, a profit of 12,575.93 CNY can be obtained per ton of silica fume processed. If energy consumption, equipment depreciation, sales, management, labor, and environmental treatment costs are reasonably controlled, the process is expected to yield good economic benefits.