Microstructure of geopolymer accounting for associated mechanical characteristics under various stress states

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1. Introduction

Geopolymer is a fine material with engineering characteristics that are similar to those of cement and concrete, but unlike ordinary Portland cement, geopolymer can be produced at low temperature [1–3]. The novel features of this “green” material include its early developed strength, high-temperature resistance, and acid/alkali resistance [4–7]. In the last decade, various mixtures used in preparing geopolymer, and the mechanical parameters of the produced specimens, have been extensively studied to compare their microstructures and engineering characteristics [8–14].

Geopolymer has an amorphous-to-semi-crystalline microstructure and a three-dimensional aluminosilicate structure that resembles those in zeolite [1,2,15]. Its forming process involves a multistage chemical reaction and yields geopolymer with a wide range of mechanical behaviors [16–18]. Many studies have investigated how composition influences its mechanical properties and have shown that the SiO2/Na2O and/or SiO2/Al2O3 mole ratios are important to the preparation of geopolymer. However, most studies have focused on the mechanical behavior of geopolymer in a uniaxial compressive stress state and have qualitatively described how structural coordination accounts for its strength. The mechanical behavior of geopolymer, including the stress–strain curves and the failure modes in various stress states, should be comprehensively tested and so the causes of variations in the mechanical characteristics and their mechanisms require further investigation.

In this study, a series of uniaxial and triaxial compressive tests of the geopolymer with various SiO2/Na2O mole ratios were performed to investigate the mechanical behavior of geopolymer in distinct stress states and how it is affected by the SiO2/Na2O mole ratio. The microstructures of these specimens are also analyzed to find out how their constituents affect the mechanical characteristics of geopolymer. The characteristics of the stress–strain curve, the failure mode in various stress states, and associated mechanisms, are clarified to improve the engineering properties of geopolymer.

2. Experimental design

2.1. Materials and specimen preparation

In this study, geopolymer is made using metakaolin, reagent-grade NaOH, industrial sodium silicate solution and deionized water. Metakaolin with a D50 of 4.29 μm is calcined from kaolin at 700 °C for 3 h. Table 1 presents the chemical compositions of adopted kaolin, which is originated in Georgia, USA. Sodium silicate solution with an SiO2/Na2O mole ratio of 3.19, viscosity < 0.01 Pa s, specific gravity of 1.12 and Antoine Baumé of 15 °Bé is used. The NaOH and deionized water are firstly mixed and left to stand for at least 3 h to induce
exothermic reactions. The geopolymer is then prepared with various SiO2/Na2O mole ratios by regulating NaOH. Specimens with SiO2/Na2O mole ratios of 1.27 to 1.91 are labeled A to F, respectively. Table 2 lists the mix proportions for each specimen in this study.

The NaOH solution and sodium silicate solution are mixed by stirring for 15 min to yield the required SiO2/Na2O mole ratios (Table 2). Once the exothermic reaction is complete, the solution is mixed with powdered metakaolin. This mixture is stirred for 20 min and then cast into a specimen mold with a diameter of 54 mm and a height of 130 mm. A shaking table is used to remove the air from specimens. Cast specimens are then kept in an oven at 25 °C at a relative humidity of 90% for 72 h. The geopolymer specimens are then removed from the molds and further cured in the same environment for 11 days. Each specimen for mechanical tests has a curing age of 14 days totally since prepared.

2.2. Test and analysis

Tests on geopolymers in this study are classified by their physical properties, mechanics, and microstructures. The physical test encompasses a general physical index such as bulk density, specific gravity, porosity, water absorptivity and wave transmittance characteristics.

To determine the mechanical parameters of the geopolymer in various stress states, both uniaxial and triaxial compressive tests are performed. Fig. 1 plots the stress paths in the uniaxial and triaxial compressive tests. The horizontal axis (p) and ordinate axis (q) respectively represent the mean of the maximum and minimum principal stresses at failure, \( p = \frac{1}{2}(\sigma_1 + \sigma_3) \), and half of the difference between the maximum and minimum principal stresses at failure, \( q = \frac{1}{2}(\sigma_1 - \sigma_3) \). In the uniaxial compressive test, the confining stresses were always zero and in the triaxial compressive test, they were 2, 4, 8 MPa until the failure of the geopolymer in various stress states. For each designed SiO2/Na2O mole ratio, at least five cylindrical specimens are tested. Deviatoric stress, i.e., the maximum principal stress subtracting the mean of principal stresses in the uniaxial and triaxial compressive tests, is applied in a displacement-controlled mode with a loading rate of 1 mm/min.

The plastic deformation before peak strength in some specimens is observed after unloading to approximate half loading following by reloading twice or thrice while deviatoric stress is applied. The peak strengths obtained in various testing stress states are used to determine strength parameters, including uniaxial compressive strengths (UCS), apparent cohesion (c) and apparent friction angle (\( \phi \)). For various confining stresses, the deformation moduli (\( E_{50s} \)) are obtained from the slopes of stress–strain curves that are measured from the origin to half of the peak strength.

The microstructures of geopolymers are analyzed using X-ray diffraction (XRD), scanning electron microscopy (SEM) and nuclear magnetic resonance (NMR) spectroscopy. The X-ray powder diffractometer is recorded at a scanning rate of 4°/min from 5° to 90° with an interval of 0.02°. Fractured surfaces selected from crashed samples of geopolymer for SEM analysis are sputtered with Au before observations are made. Low acceleration voltage (15 kV) is adopted to reduce the charge effect caused by low conductive samples. In the NMR analysis, the rate of capsule spinning is set to 10 kHz and the 27Al and 29Si spectra are measured and recorded at frequencies of 104.27 and 79.50 MHz, respectively.

3. Test results for mechanical parameters and microstructures

Table 3 lists the physical indices for each specimen. Bulk density and apparent specific gravity range 0.99–1.10 g/cm³ and 2.41–2.53 g/cm³, respectively. Porosity and water absorptivity are 54.2–60.9% and 49.1–61.8%, respectively. Except the specimen E, the physical indices for other specimens differ limited. However, the P-wave velocity (\( V_p \)) of geopolymer, ranging 1089–2430 m/s, decreases obviously as the SiO2/Na2O mole ratio increases.

3.1. Uniaxial compressive test

Fig. 2 shows the UCSs of geopolymers that are formed at various SiO2/Na2O mole ratios. The UCS is 35.9 MPa at maximum value when the SiO2/Na2O mole ratio is 1.27 (specimen A) and is only 7.6 MPa when the SiO2/Na2O mole ratio is 1.72 (specimen E). The UCS of specimen F made of an SiO2/Na2O mole ratio of 1.91 is not considered here because the peak strength cannot be determined from the stress–strain curve until the strain exceeded 3%. The UCS of the geopolymer falls as the SiO2/Na2O mole ratio increases. Fig. 3 plots the \( E_{50s} \) of geopolymers that have various SiO2/Na2O mole ratios. Specimen A has the highest \( E_{50s} \) of 2.3 GPa, and specimen E has the lowest \( E_{50s} \) of 1.0 GPa. The deformation modulus of specimen F, which approximates 0.17 GPa, is not considered here.

![Fig. 1. Stress paths in uniaxial and triaxial compressive tests.](image1)

### Table 1

Chemical compositions of adopted kaolin.

<table>
<thead>
<tr>
<th>SiO2</th>
<th>Al2O3</th>
<th>TiO2</th>
<th>Na2O</th>
<th>Fe2O3</th>
<th>MgO</th>
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<tr>
<td>wt.%</td>
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<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>44.50</td>
<td>39.50</td>
<td>1.00</td>
<td>0.52</td>
<td>0.50</td>
<td>0.07</td>
<td>0.05</td>
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### Table 2

Mix proportions for each specimen.

<table>
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<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
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<td>SiO2/Na2O</td>
<td>1.27</td>
<td>1.39</td>
<td>1.51</td>
<td>1.62</td>
<td>1.72</td>
<td>1.91</td>
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<tr>
<td>Na2O/H2O</td>
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<td>0.14</td>
<td>0.13</td>
<td>0.12</td>
<td>0.12</td>
<td>0.11</td>
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<td>7.40</td>
<td>6.67</td>
<td>5.99</td>
<td>5.44</td>
<td>4.45</td>
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<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>MK (g)</td>
<td>170</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Sodium silicate solution (g)</td>
<td>130</td>
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</tbody>
</table>

### Table 3

Physical indices for each specimen.

<table>
<thead>
<tr>
<th>Specimen</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
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</thead>
<tbody>
<tr>
<td>Bulk density (g/cm³)</td>
<td>1.10</td>
<td>1.10</td>
<td>1.09</td>
<td>1.09</td>
<td>1.08</td>
<td>0.99</td>
</tr>
<tr>
<td>Specific gravity</td>
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<td>2.41</td>
<td>2.45</td>
<td>2.47</td>
<td>2.48</td>
<td>2.53</td>
</tr>
<tr>
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<td>55.4</td>
<td>54.2</td>
<td>55.5</td>
<td>56.1</td>
<td>56.9</td>
<td>60.9</td>
</tr>
<tr>
<td>Water absorptivity (%)</td>
<td>50.3</td>
<td>49.1</td>
<td>51.0</td>
<td>51.8</td>
<td>52.4</td>
<td>61.8</td>
</tr>
<tr>
<td>( V_p ) (m/s)</td>
<td>2430</td>
<td>2307</td>
<td>1872</td>
<td>1816</td>
<td>1607</td>
<td>1089</td>
</tr>
</tbody>
</table>
decrease as the SiO₂/Na₂O mole ratio increases demonstrates that polymerization induces bonding force in the microstructure of the geopolymer specimen, which represents the completion of polymerization, decreases as the SiO₂/Na₂O mole ratio increases \[3,11–13,19\]. The effects of SiO₂/Na₂O mole ratio on developed microstructure and associated mechanical characteristics of geopolymer will be discussed later in Section 4.

Fig. 4 plots the stress–strain curves of geopolymers with various SiO₂/Na₂O mole ratios. These curves can be classified into three categories by peak strength and plastic deformation before peak strength. In the type I curve, the stress–strain has a clear peak and minimal plastic deformation before the peak. The curve is concave when the load is low and is convex close to the peak. The stress–strain curve is conspicuously linear and the slopes are very similar under loading, unloading and reloading conditions. Geopolymers that are formed at SiO₂/Na₂O mole ratios of 1.27, 1.39, and 1.51 (specimens A, B, and C) can be classified as those of type I. The type II stress–strain curves (specimens D and E) have peaks and near which they are significantly convex. These stress–strain curves are linear nearby half of peak strength, but the slopes in unloading and reloading stages exceed those in the loading stage. The type III stress–strain curve (specimen F) has no peak at least until the axial strain exceeds 3%. The stress–strain curve is nonlinear, and significant plastic deformation occurs while unloading.

3.2. XRD and SEM analyses

Fig. 5 shows the powder X-ray diffraction patterns of geopolymers that were formed at SiO₂/Na₂O mole ratios of 1.27 (specimen A), 1.62 (specimen D), and 1.91 (specimen F), respectively. The wide diffraction humps of the XRD for geopolymers (15–35°) demonstrate their semi-crystalline and amorphous structures \[20\]. All specimens yielded local peaks that were identified as quartz and un-dissolved kaolin. The diffractogram peak of specimen A in the range 15–35° was more intense than those of specimens D and F, and the local peaks associated with quartz and kaolin were lower. These results demonstrate that preparing geopolymer in a high alkaline environment, in which metakaolin is highly soluble, provides sufficient Si and Al ions to form aluminosilicate units, promoting geopolymerization.

Fig. 6 shows the SEM micrographs of specimens A, D, and F. The configuration of geopolymer components in transition stage — the
aluminosilicate particles and the gel phase are visible in all specimens, with large microstructural changes caused by polymerization at SiO$_2$/Na$_2$O mole ratios of 1.27 to 1.91. The microstructures of specimens (D and F) with SiO$_2$/Na$_2$O mole ratios $\geq 1.62$ exhibit large interconnected pores among loosely piled up aluminosilicate particles and unreacted materials. In contrast, specimen A (SiO$_2$/Na$_2$O $< 1.62$) contains an integrally homogeneous binder with small (several microns) disconnected pores and limited unreacted materials. Notably, when specimen F is formed under poor polymerization conditions (Fig. 6e), the XRD diffraction pattern in Fig. 5 reveals a considerable amount of raw metakaolin.

3.3. $^{27}$Al and $^{29}$Si NMR

Fig. 7 presents the results of $^{27}$Al NMR analyses of specimens A, B, C, and D. The figure presents the $^{27}$Al NMR chemical shifts of 4-coordinated Al(IV) and 6-coordinated Al(VI), which are 58 and 4 ppm, respectively [21]. The hump at approximately 27 ppm which indicates the 5-coordinated Al is not obvious because of the incomplete polymerization of metakaolin [22]. Magnified graphs of the chemical shifts of Al(IV) and Al(VI) reveal that for each specimen, the intensity associated with Al(IV) increases upon polymerization while that associated with Al(VI) decreases, indicating that Al(VI) is converted to Al(IV). A comparison of Figs. 2, 4, and 7 reveals that a geopolymer with a low SiO$_2$/Na$_2$O mole ratio yields a strong Al(IV) signal and a weak Al(VI) signal, and exhibits high UCS. The high OH$^-$ concentration in the mixture with the low SiO$_2$/Na$_2$O mole ratio helps to destroy the Al(VI) structure in metakaolin and the dissolution of Al ions promoting the rearrangement of AlO$_4$ and SiO$_4$ in the subsequent polymerization, yielding a well-developed three-dimensional Si–O–Al framework of the geopolymer [23]. After the coordination environments of the Al ions in the geopolymer were obtained by determining the $^{27}$Al NMR spectra, $^{29}$Si NMR analyses were subsequently carried out to determine their molecular configuration.

Fig. 8 presents the $^{29}$Si NMR spectra of all specimens. The range of NMR excitations from $-75$ to $-115$ ppm indicates the tetrahedral environment of silicon in aluminosilicate geopolymer. Specimens with type I stress–strain curves (A, B, and C) have chemical shifts that are centered at $-88.3$, $-89.0$, and $-89.3$ ppm, respectively; the shifts of

![Image of SEM analyses of specimens A, D, and F](image-url)
the specimens with type II curves (D and E) are centered at −91.1 and −91.7 ppm, respectively, and that of the specimen with the type III curve is centered at −96.0 ppm.

These widely varying chemical shifts reflect all five possible silicon Q4(mAl) structures with m = 0–4. The Si and Al cations in the framework of the aluminosilicate geopolymeric gel are tetrahedrally coordinated and linked by oxygen bridges. As the number of Si and Al bonds in a geopolymer structure is reduced, the 29Si NMR spectrum shifts toward the direction in which the magnetic field is strongest. A change in coordination of one Al atom causes a shift of approximately 5 ppm [23,24]. The chemical shifts of specimens with type I curves are centered at roughly −88 ppm, shifting to the left by about 3 ppm to approximately −91 ppm in specimens with type II curves, and by a further 5 ppm to around −96 ppm in the specimen with type III curve. The overlaps of the peaks prevent the relative positions of the peaks and the corresponding composition ratios from being directly determined from the 29Si NMR spectrum. Therefore, the fitting algorithm is utilized to separate the peaks.

Both Gaussian distribution curve and Lorentzian distribution curve can be applied for NMR signal analysis, and are popular in literature [25,26]. In this study, the Gaussian fitting, Lorentzian fitting and their combination and convolution as well have been tried to determine the five possible silicon Q4(mAl) structures. The peak positions and widths of the five Q4(mAl) structures for fitting refer to well-documented values initially [27,28] and are allowed to shift while fitting. A fitting curve is then drawn with a threshold for the coefficient of determination $r^2 > 0.9999$. Fig. 9 shows a typical observed 29Si NMR signal (specimen A) and fitting result. The Gaussian fitting algorithm is adopted for subsequent analysis since all fitting results resemble each other for specimen A. Fig. 10 shows the area of the fitting curves that corresponds to the various Al coordinations of specimens A, D, and F. The area is normalized to that of the original NMR curve and given as a percentage thereof. The SiO2/Na2O mole ratio that is used in preparing geopolymer greatly affects the degrees of polymerization of the dissolved species in an alkaline silicate solution and the resulting coordination in its structure [23,24]. Specimen A comprises mainly Q4(4Al) with an area percentage of 38%, and Q4(3Al) and Q4(2Al) with area percentages of 28% and 20%, respectively. Specimen D comprises Q4(3Al) with an area percentage of 38%, and Q4(2Al) and Q4(4Al) with area percentages of 24% and 18%, respectively. Specimen F is composed of 39% Q4(3Al), 31% Q4(2Al) and 12% Q4(4Al). For the considered range of mixtures, the use of a lower SiO2/Na2O mole ratio in the preparation of the geopolymer causes a higher proportion of Q4(4Al) to form in its structure; resulting in a greater UCS. Analyses of 27Al and 29Si NMR also reveal that, as the SiO2/Na2O mole ratio used to prepare geopolymer increases, the proportions of developed Q4(1Al), Q4(2Al), and Q4(3Al) increase, and the UCS decreases. The proportion of Q4(4Al) affects the strength of the geopolymer.

3.4. Triaxial compressive test

Based on the observed deformation and the spatial distribution of the rupture surface in the specimens, the failure patterns of the geopolymer in various stress states can be identified as consistent
with five modes; (1) split (SP), with at least one rupture surface distributed vertically, occasionally accompanied by a crumbling surface; (2) split accompanied by sheared failure (SS), with vertical rupture surface(s) connected by inclined sheared plane(s); (3) monoclinic sheared failure plane (MS), typically with a single inclined sheared surface; (4) conjugate sheared failure planes (CS), and (5) ductile deformed failure (DD), with significant deformation of the specimen upon failure. Table 4 summarizes the failure modes of specimens following uniaxial- and triaxial compressive tests, along with typical photographs of these failure modes.

Figs. 11–13 plot the stress–strain curves of specimens A, D, and F, respectively, under various confining pressures. The peak strength and corresponding strain of specimen A increase with the confining pressure (Fig. 11). Under the tested confining pressure states, all of the stress–strain curves are concave in the initial loading stage and convex as the loading approaches the peak strength. The convex section of the curve becomes wider as the confining pressure increases, and the failure mode shifts from SP to SS, which is the characteristic of a brittle material. The stress–strain curves of specimen D resemble those of specimen A, especially in terms of peak strength, when \( \sigma_3 < 4 \text{ MPa} \) (Fig. 12). However, when \( \sigma_3 \geq 4 \text{ MPa} \), the range of the convex section considerably increases, and the peak strength is unclear. The stress–strain curves of specimen D are characteristic of ductile materials, and the failure modes shift from SS in the uniaxial compressive state to SS + MS (\( \sigma_3 = 2 \text{ MPa} \)), MS + CS (\( \sigma_3 = 4 \text{ MPa} \)), and CS as \( \sigma_3 = 8 \text{ MPa} \) as \( \sigma_3 \) is increased. The characteristics of the stress–strain curves and failure modes vary dramatically with the testing confining pressure. The stress–strain curves of specimen F have completely different characteristics from those of specimens A and D (Fig. 13). When a limited deviatoric stress is applied, significant strain is observed, but the peak strength cannot be determined before the strain reaches 10% when \( \sigma_3 = 0 \) and 2 MPa. The specimen is deformed during tests with a significant reduction in volume and a DD failure mode when \( \sigma_3 = 2 \) MPa. Several transverse failure planes perpendicular to the direction of deviatoric stress are identified at the end of triaxial compressive test. The specimen is thus determined too weak to sustain a confining pressure of 2 MPa, so failure occurs when a confining pressure is applied but not thereafter when a deviatoric stress is applied.

The specimens that are formed with various SiO\(_2\)/Na\(_2\)O mole ratios have high peak strengths and a correspondingly large failure strain when a high confining pressure is applied in the triaxial compressive tests. However, they have greatly different deformation moduli. Fig. 14 presents the deformation moduli of all specimens under various confining pressures. The \( E_{50s} \) decreases as the SiO\(_2\)/Na\(_2\)O mole ratio that is used in the preparation of the geopolymer increases under all confining pressures. Furthermore, the \( E_{50s} \) of specimen C varies slightly with the confining pressure. For specimens D and E, which are prepared with SiO\(_2\)/Na\(_2\)O mole ratios greater than that of specimen C, the \( E_{50s} \) consistently decreases as the confining pressure increases. For specimens A and B, which have an SiO\(_2\)/Na\(_2\)O mole ratio that is lower than that of specimen C, the \( E_{50s} \) increases with confining pressure up to \( \sigma_3 = 2 \text{ MPa} \) and then decreases as confining pressure increases further.

4. Discussion

The results of uniaxial compressive tests show that geopolymers with various SiO\(_2\)/Na\(_2\)O mole ratios undergo different polymerizations, and therefore exhibit various mechanical behaviors. The geopolymer that has undergone complete polymerization has a type I stress–strain curve. This geopolymer has a well-developed microstructure with few pores and exhibits linear elastic deformation under uniaxial compressive loading. The type I specimen is split into flakes or pieces in failure mode (Table 4). The geopolymer with insufficient polymerization has a type II stress–strain curve. A macrostructure with defects, such as large pores and an incompletely developed aluminosilicate structure, results in considerable deformation during uniaxial compressive loading, and plastic deformation while unloading. The specimen of type II generally fails by crack propagation with typical inclined shear failure surface(s). The geopolymer with poor polymerization has a type III stress–strain curve, resembling that of raw materials, such as soil-like metakaolin. Failure in this specimen is caused by conjugate shear cracking and large deformation. Notably, the geopolymer specimens prepared in this study, except specimen E, have similar bulk density, specific gravity, porosity and water absorptivity.

### Table 4

Failure modes and associated characteristics of geopolymers.

<table>
<thead>
<tr>
<th>Failure modes</th>
<th>Description</th>
<th>Symbol</th>
<th>Photographic Depiction</th>
<th>Photograph</th>
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<tr>
<td></td>
<td></td>
<td>SP</td>
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<td>SS</td>
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<tr>
<td></td>
<td></td>
<td>DD</td>
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</tr>
</tbody>
</table>

[Fig. 11. Stress–strain curves of specimen A in triaxial compressive test.]
Table 5 lists the failure modes for all specimens under various confining pressures. Specimens in the uniaxial confining state with types I, II, and III stress–strain curves fail with SP, SS, and SS + CS modes, respectively. As the confining pressure increases, the failure modes for the specimens with the type I curves shift from SP to SS and MS. Among these specimens, specimen A, which is the specimen with greatest peak in this study, suffers SP and SS failure with a few rupture planes, and specimens B and C fail with MS when \( \sigma_3 \geq 4 \text{ MPa} \). The failure modes of the specimens with the type II curves vary with the confining pressure, shifting from SS in the uniaxial compressive state to CS at \( \sigma_3 = 8 \text{ MPa} \), with modes SS + MS, MS + CS, and MS in between. The specimen with the type III curve has failure mode SS + CS in the uniaxial compressive state and DD when \( \sigma_3 = 2 \text{ MPa} \). The triaxial compressive test of the specimen with the type III curve ends at \( \sigma_3 = 2 \text{ MPa} \) owing to its poor strength.

Fig. 15 plots the failure envelopes in \( p-q \) stress space for all specimens. The strength parameters in \( p-q \) stress space were determined by linear regression analysis and then converted to corresponding parameters to determine whether the Mohr–Coulomb failure criterion was met. The coefficients of determination \( r^2 \) have a minimum of 0.95, indicating that the linear failure envelope effectively describes the stress failure of the geopolymer and the test results of the uniaxial- and triaxial compressive tests are mutually consistent.

Fig. 16 plots the variation of strength parameters of geopolymers that were formed at various SiO2/Na2O mole ratios. The apparent cohesion was highest, 8.32 MPa, for specimen A, slowly decreasing as the SiO2/Na2O mole ratio that was used in the preparation of the geopolymer increased, reaching a minimum of 0.53 MPa for specimen F. The apparent friction angle follows a two-stage increasing curve connected with a decreasing section. The apparent friction angle of the specimens with the type I curves increases with the SiO2/Na2O mole ratio. However, the apparent friction angle noticeably decreases when the SP failure mode disappears in uniaxial compressive state and the CS emerges as \( \sigma_3 \) rises above 4 MPa. The apparent friction angles of specimens with type II and III curves increase with the SiO2/Na2O mole ratio. Notably, specimen F is too weak to sustain triaxial compressive stress as \( \sigma_3 > 2 \text{ MPa} \), limiting the range of results that can be obtained from tests to determine the strength parameters and possible deviations from associated representative values.

In summary, the SiO2/Na2O mole ratio that is utilized in preparing a geopolymer critically affects the completion of polymerization, resulting in various coordinations in the aluminosilicate structure. The coordination in the aluminosilicate structure determines the mechanical behavior of the geopolymer. However, the specimens that are prepared in this study are not perfectly coordinated aluminosilicate structures. They have distinct silicon Q4(mAl) structures. Accordingly, these specimens are very sensitive to changes in the magnitude of confining pressure during the triaxial compressive test and so exhibit rather different mechanical behaviors.

Specimens that are prepared with SiO2/Na2O mole ratios \( \geq 1.91 \) (specimen F) behave similarly to normally consolidated clay because their change of microstructure upon geopolymerization is smaller than that of the original aluminosilicate structure. Therefore, the raw material, kaolin, dominates their mechanical characteristics. The specimens that are prepared with SiO2/Na2O mole ratios \( \leq 1.72 \) are formed by geopolymerization and so aluminosilicate structures are formed by the changing of coordinations. Of these, specimens D and E have defects in their structures owing to incomplete polymerization, and they behave like over-consolidated clay or soft weak rock. The other specimens, A, B, and C, have better development for aluminosilicate

<table>
<thead>
<tr>
<th>Specimen</th>
<th>SiO2/Na2O</th>
<th>( \sigma_3 )</th>
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<th>2</th>
<th>4</th>
<th>8</th>
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<tbody>
<tr>
<td>A</td>
<td>1.27</td>
<td>SP</td>
<td>SS</td>
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<td>B</td>
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<td>SP</td>
<td>SS</td>
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structures, and their linear elastic behavior under a low confining pressure and their moderate plastic deformation under a high confining pressure reveal that their mechanical behaviors are similar to those of rocks with weak to moderate strength.

5. Conclusions

A series of mechanical and microstructural investigations reveal that the SiO2/Na2O mole ratio that is used in preparing geopolymer with similar physical properties affect the polymerization, mainly by determining in the forms of Q4(mAl) coordinations, generating geopolymers that contain various proportions of silicon Q4(mAl) structures.

1. The well-developed geopolymer features brittle failure under uniaxial compressive state. With the raise of confining pressure in triaxial compressive test, the failure strain increases and the specimen changes to be slightly ductile. The failure modes of geopolymer with various geopolymerization range from split (SP), split accompanied by shear failure (SS), monoclinic shear failure (MS), conjugated shear failure (CS) and ductile deformed failure (DD).

2. The proportions of Q4(mAl) coordinations account for the sensitivity of the response of the geopolymer to various confining pressures. The proportion of Q4(AlA) correlates positively with the mechanical characteristics of geopolymer and correlates negatively with Q4(2Al).

3. Incomplete polymerization generates geopolymer with an imperfect microstructure, which explains the plastic deformation that is observed during unloading. The polymerization processes for the geopolymer are responsible for its apparent cohesion and apparent friction angle. Nevertheless, the friction-induced strength dramatically decreases when the failure mode of specimens shifts from the split mode to the shear mode.

Acknowledgments

The authors would like to thank the National Science Council, Taiwan, for financially supporting this research under Contract Nos. NSC 97-2621-M-027-003 and NSC 101-3113-E-027-001.

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