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Structure and Analysis of Natural Nano Silicate Layers Based on (RM-K) Fracture Theory

EL-SHEIKHY Refat*, AL-SHAMRANI Mosleh* and KOBAYASHI Akira**

Abstract

Current research is intended to study the structure phenomenon of natural nano silicate layers. The research studies the effect of water on the structure of the material and also, the stresses due to the effect of drying of the material. The research includes a study of the change of structure, fracture, cracking mechanism, crack propagation, crack branching and bifurcations. The results conclude that the silicate layers are very sensitive to temperature. Cracks and fracture will be produced due to the loss of water due to shrinkage as the effect of heat loss or temperature changes. One of the most important properties of the nano silicate is the hydrophilic property. This property makes it very sensitive for absorbing water or losing it. As a result of absorbing water the silicate volume changes by swelling while due to loss of water or drying the silicate will shrink. If the silicate is dried, it will be fractured. It is found that if the nano silicate is added to another matrix material representing filler or reinforcement for that main material temperature stability and temperature resistant material. If it is mixed with polymers under certain conditions it can produce high quality material of nanocomposite. A mechanism of silicate cracking is proposed. A new and special version of directional fracture theory called (RM-K) theory is proposed for the application of silicate cracking since it follows different behavior than the normal fracture approach.

KEY WORDS: (Nano silicate), (Structure), (Analysis), (Swelling), (Shrinkage), (Cracking), (RM-K fracture theory)

1. Introduction

In the last few years nanocomposites have been attracting much attention as materials with great benefits. This is because nanocomposites exhibit unique properties and functions which are different from those of conventional materials. Due to this unique structure as natural layered nano materials, rich chemical intercalation and low cost, clay minerals are promising reinforcements or filler material for polymers to manufacture low-cost, lightweight and high performance nanocomposites. Therefore, this research project is designed to use clay particles to produce clay-based polymer nanocomposites using Saudi Arabian domestic materials.

Many researchers during the last decade studied clay mineral nano platelets mixed with polymers to produce nanocomposites. Some researchers studied the processing [1-16] while others concentrated their research on characterization [17-25]. Other researchers studied fracture of the clay based nanocomposites. The modeling and morphology were also studied by many researchers. The thermal and flammability properties were studied in addition to gas barrier properties. All previous studies faced several difficulties. The major difficulties facing

the development of clay-based polymer nanotechnology are the lack of understanding of the mechanisms. Although many researches for modeling have been carried out for understanding the mechanisms of enhancement of engineering and physical properties for clay base -polymer nanocomposites, they have far from solved the problems. For example, the exact mechanical properties of individual silicate layers are not known. Therefore, it is difficult to develop a mechanism of fiber reinforcement. The mechanism and strength of bi-interfaces of clay-polymer nanocomposites is not yet clear. Extensive modeling and fundamental experimental research should be conducted to solve these problems.

This research project is prepared for studying the clay-based polymer composite which is classified as a nanocomposite. Since the composite material can be classified as a nanocomposite if it contained at least one component having at least one dimension equal 1.0 nm as in the case of clay mineral platelets or two nano dimensions like carbon nano tubes or three nano dimensions like spherical particles. Clay nano platelets which may be natural or synthesized, it has several unique advantages such as low price, inorganic, friend of nature, chemically intercalated and high strength. Nano clay is hydrophilic and thermoset material. Inside

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polymer matrix, the dispersion and exfoliation of clay nano platelets are difficult processes in addition to the distribution intensity. Also, nano clay platelets are orientation uncontrolled. Our study will consider these important aspects. The project is mainly designed for the fundamental mechanics analyses and experimental verification to solve the difficulties of previous work [1-25].

Previous works could not investigate the most important aspect of the clay based polymer nanocomposites. Therefore this research is conducted mainly for developing the clay based nanocomposite. Extensive studies have been made on this field but could not solve any of these problems. The factors governing the strength and the required properties on the nanocomposite are the original properties of the composite components such as mechanical properties, structure, and fracture properties, thermal and chemical properties. This research will include experimental and theoretical works. Experimental work will include processing, characterization and testing while the theoretical work includes concept, approach, modeling, mechanism, analyses and comparisons. The directional strain energy approach will be applied regarding the energy components. It will consider size, and shape effects. The study will be carried out on two or three types of clays and polymers.

2. Nano Silicate Structure

Clays have several properties which can be considered as unique natural phenomena such as:

- 1- Clay is a hydrophilic material which makes it very sensitive water absorption or loss under thermal effects or the effects of external loads.
- 2- Swelling phenomenon due to water absorption producing volume change of the clay with high ratio.
- 3- The swelling weaken the bonds between clay layers.
- 4- High surface area due to the nano size thickness and high aspect ratio.
- 5- Shrinkage due to loss of the water by the thermal effect.
- 6- Fracture and cracking due to shrinkage phenomenon.
- 7- The fracture which is internal due to shrinkage is 3-D fracture with 3-D bifurcations and branching.
- 8- Each separation of the clay layers by breaking the bond between clay layers.
- 9- High properties such as strength, thermal stability, gas and water barrier, thermal stability, etc.
- 10- These properties are very important for many applications such as drugs, medicines, nanocomposites, gas barriers, coatings, electric devices, electronics, automobiles, aircrafts, etc.

The study will focus on the structure, forces and

cracks due to shrinkage since the most important and dangerous phenomenon of the clay is shrinkage.

3. Nano Silicate Based - Nanocomposite

The natural structure of clay makes it a unique material since it has a structure different from all other materials. There are many types of clay which have different structures with different dimensions and properties. In general, a clay mineral consists of silicon layers of tetrahedral structure connected to octahedral aluminum layers as shown in **Fig.2**. The montmorillonite type (MMT) consists of two layers of silicon sandwiching one layer of aluminum as shown in **Figs.1-6**, while the Kaolinite type consists of two layers of octahedral aluminum; sandwiches one tetrahedral layer of silicon. These three layers are always found connected to another three layers through another material which has positive electric charge such as Mg, K, Na, or Ca because the clay particles have negative charge. The clay layers are always found in agglomerated particles. Clay has the property of cations exchange capacity CEC since clay layers have (-ve) charge. Therefore, it can exchange cations with (+ve) charged particles of Mg, K, Na and Ca. Therefore, bonds of clay layers depend on the ionic bond. In addition, there are other bonds such as Van der Waals and covalent bonds. The surface area of the clay is

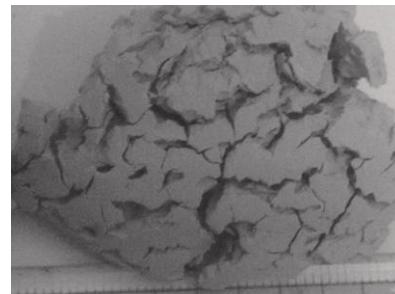


Fig.1 Natural Saudi MMT fractured under shrinkage with different types of cracks.

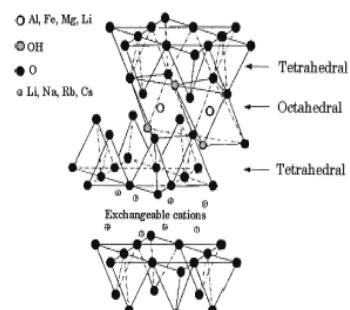


Fig.2 Structure of MMT.

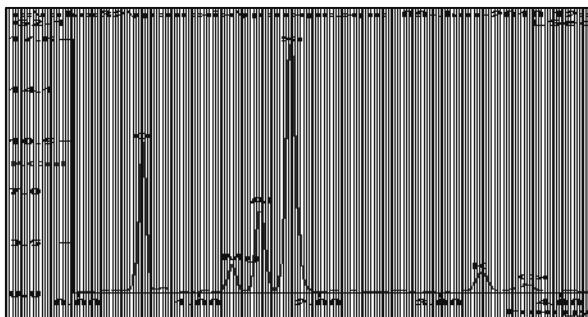


Fig.3 Edax analysis of Saudi MMT.

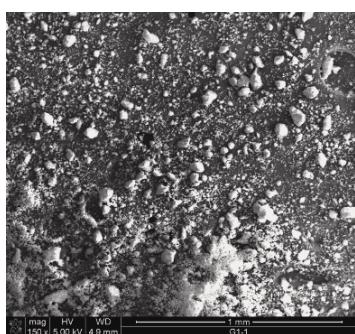


Fig.4 Agglomerated particles of Saudi MMT.

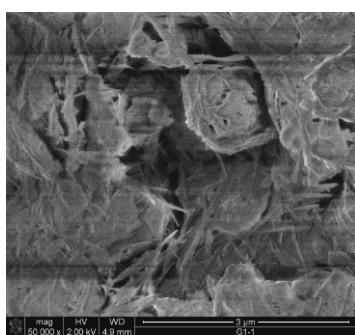


Fig.5 SEM image showing fibers of agglomerated Saudi MMT.

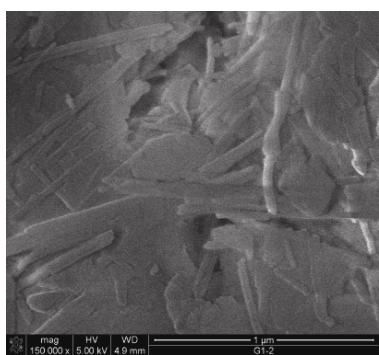


Fig.6 SEM image showing fibers of one type of Saudi MMT.

very high since the aspect ratio is very high. The clay thickness is about 1.0 nm for MMT, while it varies for other types with thickness larger than 1.0 nm while the length is about 100 nm – 5 μ m.

Current research is intended to study the structure phenomenon of natural nano silicate layers. The research is done by studying the effect of water on the structure of the material and the stresses due to the effect of drying of material which will produce stresses due to shrinkage. The research includes the study of the change of structure, fracture, cracking mechanism, crack propagation, crack branching and bifurcations. The results conclude that the silicate layers are very sensitive to temperature. Cracks and fracture will be produced due to the loss of water due to shrinkage as the effect of heat loss or temperature changes. One of the most important properties of the nano silicate is its hydrophilic property. This property makes it very sensitive for absorbing water or losing it. As a result of absorbing water the silicate volume changes in swelling phenomenon while due to loss of water or drying the silicate shrink. If it is dried the silicate will be fractured. It is found that if the nano silicate is added to another matrix material representing a filler or reinforcement for that main material, temperature stability and temperature resistance are improved. If it is mixed with polymers under certain conditions it can produce high quality materials of nanocomposite. The mechanism of silicate cracking is proposed. A new and special version of directional fracture theory called (RM-K) theory is proposed for the application of silicate cracking since it follows a different behavior from the normal fracture approach.

4. Analysis

4.1. Nanosilicate structure

Figures.2-6 show the structures of MMT clay layers. The clay particles cannot be found in nature in single layers or single phase since it is strongly hydrophilic material. The bonds between clay layers are due to each of Van der Waals forces, ionic bond, hydrogen bonds and covalent bonds. These bonds can be easily broken by adding water to the clay since clay is a hydrophilic material having very high capacity for absorbing water. This water can break the bonds between the layers. The bonds can also be broken by shear stresses on the clay layers but high shear stresses are needed. Due to absorbing the water clay volume will be changed through swelling. Due to drying of the clay, the clay continuum material will have many cracks due to fracture of clay. Fracture will propagate in branching or bifurcation to multi directional 3-D cracks. This phenomenon may have an advantage because it allows the clay to be added easily or oriented between each pair of the cracked layers. The clay layers are locally oriented but are very difficult to be controlled.

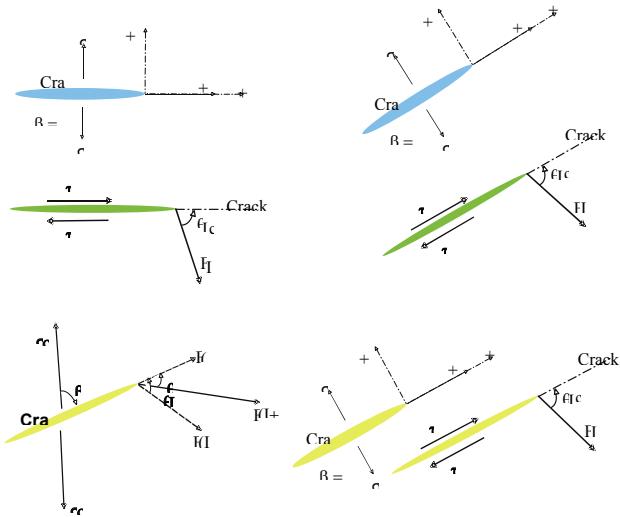


Fig. 7 Different types of cracks of silica.

4.2 Types of cracks

This research focus on the most important phenomenon in clays which is the fracture of clay layers under shrinkage stresses. As shown in Fig 1 and **Fig.7**, the cracks have many orientations. These cracks represent all different types of cracks. It may be Mode I, Mode II and mixed mode. Mode I shrinkage crack phenomenon is one of the most important results of these cracks. Another one of the most important results of these cracks which can be investigated is the benefit and advantage of the crack directions to determine the exact orientation of the clay fibers. The crack directions are in the same original directions of the clay fibers. This is for loaded clay material with shrinkage stresses. As shown in Fig.1, these cracks are intersected with each other producing network of cracks with different orientations. Some of these cracks can be branched in two or more branches or bifurcations depending on the local group orientation of clays. There is one important question raised which is "Can the fracture of Clays be controlled?" The answer is yes it can. Truly, we could succeed to control these cracks and almost prevent them to propagate or to be macroscopic in scale. This is done by using the nano technology application. This result will be published soon after more verification.

4.3 Proposed fracture theory for silicate cracks (RM-KSU) theory

One of the most important properties of the nano silicate is its hydrophilic property. This property makes it very sensitive for absorbing water or losing it. As a result of absorbing water the silicates volume changes in swelling phenomenon while due to loss of water or drying the silicate shrink. If it dried the silicate will be fractured.

The fracture and cracking will be produced

mainly due to volume change. But this volume change will be accompanied by shape change. This means that the silicates will loss volume change or what is called dilatational energy. In the same time it may loss shape change or what is called distortional energy. This means that most or all of the cracks will be under Mode I crack conditions. Therefore, the distortional energy will be the Mode I distortional energy component. But, actually the Mode I crack will be controlled by the dilatational energy. The mechanism of the fracture and cracks can be studied on the view of this theory.

1- Calculating of global fracture direction (θ_c) and global fracture load (σ_c) by means of directional volumetric-distortional strain energy theory.

2. The second step is for calculations of the local fracture direction or directions at the same points. These directions are already pre-determined by the directions and locations of bond between each two particles.

3. The local fracture load should be determined.

4. The local bond strength will be calculated in the core region near the global crack tip to find which bond will start fracture first or start together.

Usually at each crack tip there is one bond or more.

5. New crack surfaces will be produced

4.3.1 Fracture condition of propagation direction of mode I crack

Crack will propagate in the direction of maximum minimum distortional strain energy density factor ($S_{dI\min}$)_{max} when it will be in the same direction of minimum length of the plastic zone radius ($r_{PI\min}$) when in the same time pass on the plastic zone boundaries through the point of maximum value of the circumferential tensile stress ($\sigma_{\theta I\max}$).

$$\frac{\partial(\vec{s}_{dI\min})_{\max}}{\partial\theta}=0 \quad \frac{\partial^2(\vec{s}_{dI\min})_{\max}}{\partial\theta^2}\geq 0$$

4.3.2 Fracture condition of starting propagation and propagation load of mode I

Crack will start propagation when all of the three fracture factors the maximum volumetric strain energy density factor ($S_{VI\max}$), minimum radius of the plastic zone ($r_{PI\min}$) and maximum circumferential tensile stress factor ($\sigma_{\theta I\max}$) reaches their critical quantity in the same time $S_{VI} > S_{VIc}$

4.3.3 Fracture condition of propagation direction of mode II crack

Crack will propagate in the direction of minimum distortional strain energy density factor ($S_{dII\min}$) when it will be in the same direction of minimum length of the

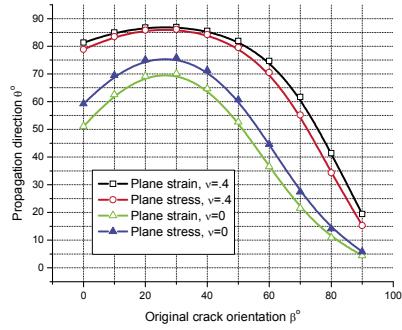


Fig.8 Relation between crack orientation and fracture direction.

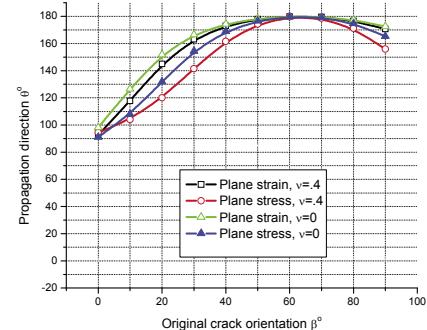


Fig.12 Relation between crack orientation and fracture direction.

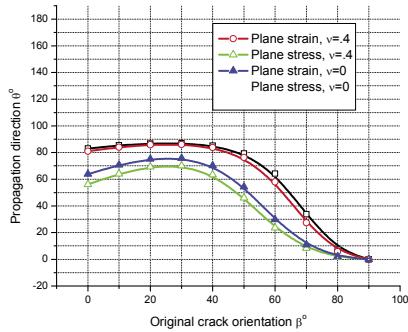


Fig.9 Relation between crack orientation and fracture direction.

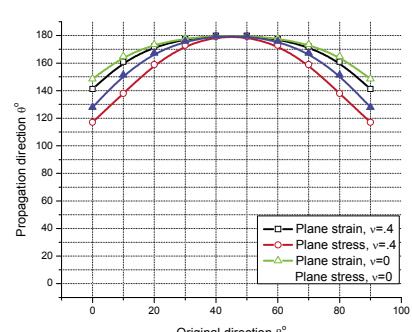


Fig.13 Relation between crack orientation and fracture direction.

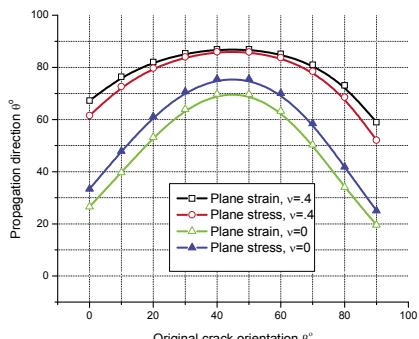


Fig.10 Relation between crack orientation and fracture direction.

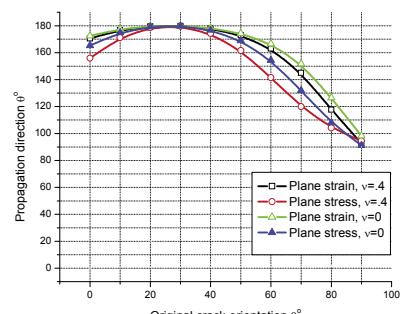


Fig.14 Relation between crack orientation and fracture direction.

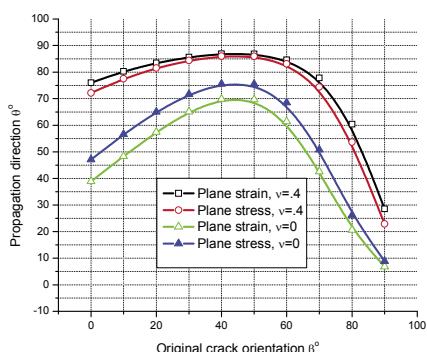


Fig.11 Relation between crack orientation and fracture direction.

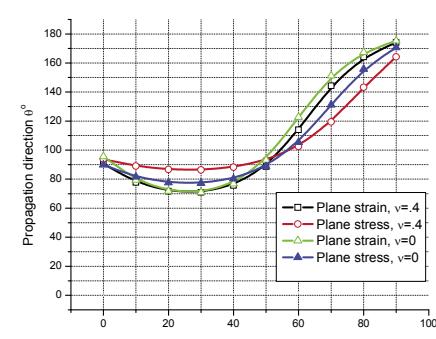


Fig.15 Relation between crack orientation and fracture direction.

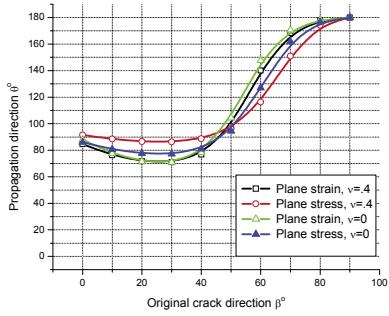


Fig.16 Relation between crack orientation and fracture direction.

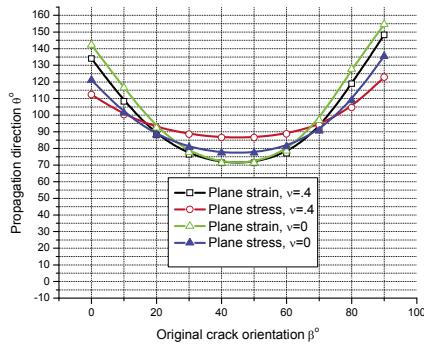


Fig.17 Relation between crack orientation and fracture direction.

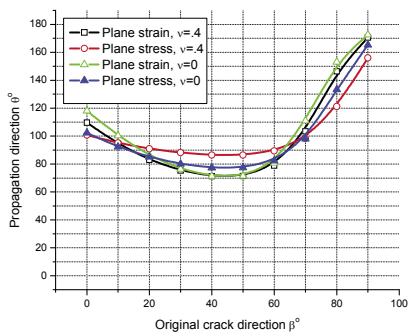


Fig.18 Relation between crack orientation and fracture direction.

plastic zone radius $r_{\text{PII min}}$ when in the same time pass on the plastic zone boundaries through the point of maximum value of the circumferential tensile stress $\sigma_{\theta\text{II max}}$.

$$\frac{\partial(\bar{s}_{d\text{II}})}{\partial\theta}_{\min}=0 \quad \frac{\partial^2(\bar{s}_{d\text{II}})}{\partial\theta^2}_{\min}\geq 0$$

4.3.4 Fracture condition of starting propagation and propagation load of mode II

Crack will start propagation when all of the three fracture factors the maximum volumetric strain energy density factor ($S_{\text{VII max}}$), minimum radius of the plastic

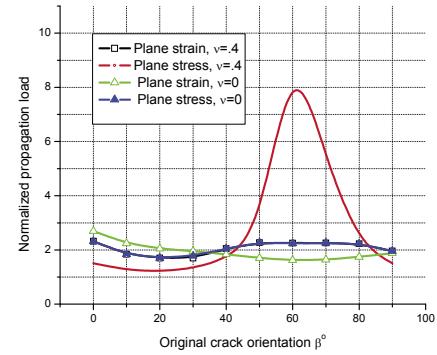


Fig.19 Relation between crack orientation and fracture load.

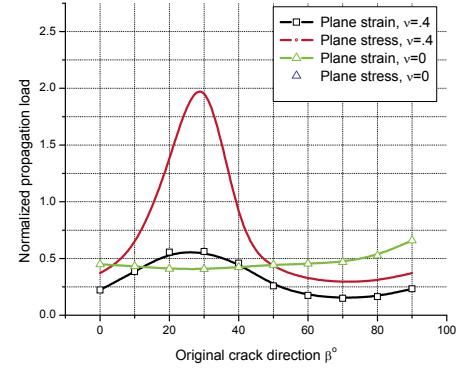


Fig. 20 Relation between crack orientation and fracture load.

zone ($r_{\text{PII min}}$) and maximum circumferential tensile stress factor ($\sigma_{\theta\text{II max}}$) reaches their critical quantity in the same time

$$S_{d\text{II}} > S_{d\text{IIc}}$$

4.3.5 Fracture condition of propagation direction of mixed mode crack

Crack will propagate in the direction of maximum minimum distortional strain energy density factor ($S_{d\text{I max}}$ $\text{min}_d\text{II min}$) when it will be in the same direction of minimum length of the plastic zone radius ($r_{\text{PI min}} - \text{PII min}$) when in the same time pass on the plastic zone boundaries through the point of maximum value of the circumferential tensile stress ($\sigma_{\theta\text{I max}} - \theta\text{II max}$).

$$\bar{s}_{d\text{I-II}}^{\text{tension}} = \left[(s_{d\text{I}} + s_{d\text{II}} \cos\theta_{\text{II}})^2 + (s_{d\text{II}} \sin\theta_{\text{II}})^2 \right]^{\frac{1}{2}}$$

$$\bar{s}_{d\text{I-II}}^{\text{compression}} = \left[(-s_{d\text{I}} + s_{d\text{II}} \cos\theta_{\text{II}})^2 + (s_{d\text{II}} \sin\theta_{\text{II}})^2 \right]^{\frac{1}{2}}$$

4.3.6 Fracture condition of starting propagation and propagation load of mixed mode

Crack will start propagation when all of the three fracture factors the maximum volumetric strain energy

density factor ($S_{VI\ max} - VII\ max$) , minimum radius of the plastic zone ($r_{PI\ min} - PII\ min$) and maximum circumferential tensile stress factor ($\sigma_{\theta I\ max} - \theta II\ max$) reaches their critical quantity in the same time

$$S_{VI-II} > S_{VI-IIc}, S_{DI-II} > S_{DI-IIc}.$$

5. Results

Figures 8-18 indicate the results of the orientation direction for different fracture cases of the cracking process of the silicate aluminum under thermal stresses of shrinkage according to continuum approach and the fracture theory (RM-K) which is depending on the directional fracture approach. Using these figures the orientation can be predicted. The stresses which are responsible on the fracture can be predicted through the conditions of the (RM-K) theory and the charts indicated in **Figs. 19-20**.

6. Conclusion

The structure, analyses, and fracture are studied. A suitable fracture theory is proposed (RM-K fracture theory). The fracture aspects are investigated under the thermal stresses of shrinkage. Characterization is done using SEM and EDAX analyses. The results are important for studying the nano silicate and nanocomposite.

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Saud Univ., Saudi Arabia.

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