Saturated dislocations transient propagation-evolution in olivine structure under ultra high-coupled thermal-force fields

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Abstract: Based on the first principle and flow driven pore-network crack theory, the crystal size saturated dislocations transient (10-4~10-5s) propagation-evolution in olivine structure under ultra high-coupled temperature (200~500°C) and pressure (0.4~1GPa) are studied on the parallel CPU&GPU platform. First, the molecular-micro scale transient fracture model is established by using hybrid hypersingular integral equation & Lattice Boltzmann method, the hydrogen ion and oxonium ion transport-dehydration (HI-OI-TD) in olivine [(FeMg)SiO4] crystal are explored. The bond-strength-length as function of thermal-force-time fields, the limited thermal-force value for HI-OI-TD through the crystal, and the ion state water adsorption in the crystal are calculated, respectively. Then, based on the above results, the crystal size saturated dislocations/defects propagation-evolution is studied. The relationship between the stress distribution and micro strain under different velocity-time conditions, the saturated dislocations/defects propagation-evolution as function of coupled thermal-force-time fields are obtained. All these findings can helpful understand the mechanism of the dehydration fracturing shale gas, the coal-gas outbursts, and the coseismic triggering issues.
Keywords: Saturated dislocations propagation-evolution; Molecular-micro transient scale fracture model; Flow driven pore-network crack model; First principle; Ionic fluid transport-dehydration; Ultra high temperature and pressure; Parallel CPU and GPU.

MECHANICS MODEL

Based on the olivine [(Fe Mg) Si O4] molecular crystal structure and micro CT tomography technology, the molecular-micro sales mechanics model can be created, respectively. Using the olivine crystal parameters in reference, the three dimensional molecular structure of olivine crystal can be obtained (Figure 1A and 1B), then applying HHIE-LBM and flow driven pore-network crack theory, the relatively molecular transient fracture model is established (Figure 1C and 1D). Figure 1C shows the mesh grid model of olivine crystal structure; the resolution at three directions is equal to molecular character length. Figure 1D shows the molecular H2O fluid flow (ionic fluid OH, hydrogen ion and oxonium ion) translate-dehydration and interaction of fluid-solid (navy blue color represents pore-flow and other colors mean sketch-solid structure). As shown in Figure 2, the relatively olivine crystal size saturated dislocations/defects transient fracture model is established by flow driven pore-network crack theory. The left part of Figure 2 is the physical model of olivine specimen and the diameter and length of the sample are equal to 5cm and 10cm, respectively. The right part of the Figure 2 is the relatively virtual physical model of olivine specimen and both resolution on cross section and interval on length direction of virtual physical model are equal to 10μm (the micro CT tomography data is done from Kochi Institute for Core Sample Research, Japan Agency for Marine-Earth Science and Technology).

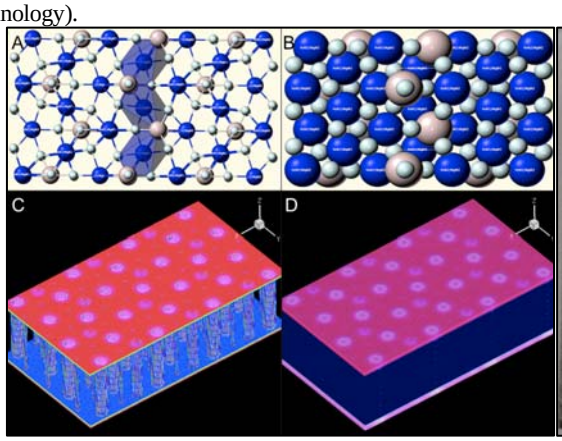

Figure.1. Olivine molecular transient fracture model

Figure.2. Olivine micro transient fracture model

NUMERICAL PROCESS AND DISCUSSION

In this section, the numerical solutions and calculations described in the present paper are used in analyzing the olivine ionic state fluid transport-dehydration and olivine micro scale saturated dislocation/defects transient propagation-evolution under coupled ultra high temperature (200~500°C) and pressure (0.4~1GPa) fields (UH-TPF) fields on the parallel CPU&GPU platforms.

5.1 The hydrogen ion and oxonium ion transport-dehydration in olivine [(FeMg)SiO4] crystal

The initial pressure and temperature are defined as 1.0GPa and 100 ºC, the hydrogen-oxonium bond-strength-length variation as function of time step is simulated. With the time increased, the bond strength is decreased and the bond length is increasing, when the time step is reach to 1800ts (1ts=10-5s), he bond length is reach to the maximize value (8~10% longer than the original length) and the bond strength is begin destruction. We can also find that the bound-strength-length is sensitive to temperature and time parameters.

So under fixed pressure 1.0GPa, the bond-strength-length variation as function of temperature [100 ºC ~550 ºC and time steps [1800ts~3600ts] are calculated and show in Figure3. At 1800 time step, when the temperature is equal to 100 ºC, the thermal vibration of molecular is located at stable state, with the temperature increased; the bond-strength-length is weaken and began to destruction at temperature 350 ºC. When the temperature is increased to 550 ºC the molecular bond strength-length is completely destroyed.

To 2400 time step, 3000 time step and 3600 time step cases, we can find that bond-strength-length is weaken with the temperature increased and is also sensitive to the duration time, even at 100 ºC temperature, the bound-strength-length is weakened and destroy with

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time step increased. When the time step is reach to 3600 time step and temperature is reached to 550 ºC, the molecular bound is very weaken and molecular is very active. At this state, the hydrogen ion and oxonium ion can transport through internal olivine crystal structure, if we increased the pressure level, the dehydration of hydrogen ion and oxonium ion in crystal will happen. All these findings are very interesting and can help us explore flow driven pore-network crack mechanism of olivine on micro-scale (at polycrystalline level).

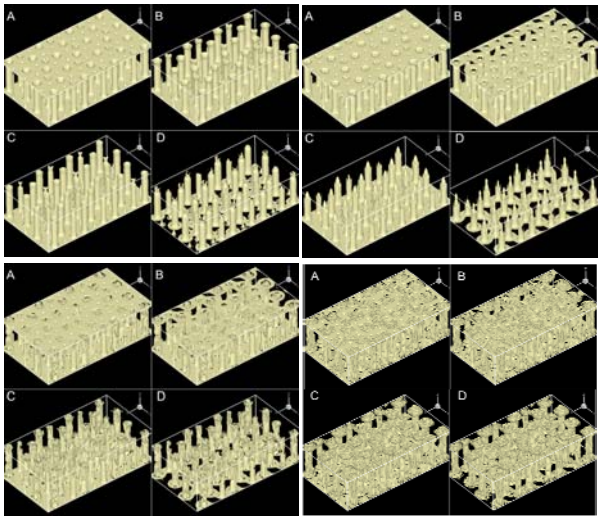

Figure.3. Bond-strength-length various as function of temperature under1.0 GPa and 1800 time step (LT-1800ts; RT-2400ts;LB-3000ts; RB-3600ts)

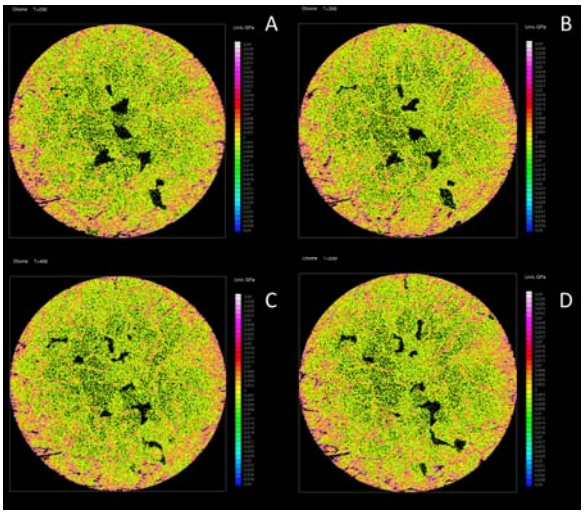

Figure.4. Olivine surface crack network plastic deformation and stress distribution as function of temperature under fixed tangential stress 0.04GPa at 500ts

5.2 The saturated dislocations/defects transient propagation-evolution under coupled thermal-force fields

Based on the above results, we can define the initial pressure and temperature condition for transient olivine crystal size dislocations/defects propagation-evolution which included the hydrogen ion and oxonium ion transport-dehydration affection. The irregular shape saturated pore-network dislocations/defects propagation with the time passed and the stress concentration distribution is far away from the large dislocation/defects. The saturated cracks evolutions are the key factor, which affect the magnitude of transient friction coefficient value.

Figure 4 shows that saturated dislocations/defects and stress distribution as function of temperature under fixed tangential stress 0.04GPa at 500ts. The crystal-induced defect propagation with the temperature increased, and the defect size and shape various with temperature changes.

CONCLUSION

In the present work, the olivine ionic state fluid transport-dehydration and olivine micro scale transient saturated pore-network dislocations /defects propagation-evolution has been explored for the first time. The following interesting findings can be drawn from our results:

1. At molecular scale, the hydrogen ion and oxonium ion transport-dehydration (HI-OI-TD) in olivine [(FeMg)SiO4] crystal are explored. The variation of bond-strength and bond-length as function of thermal, stress and time is obtained, the limited thermal-pressure value for HI-OI-TD through the internal crystal, and the ion state of water adsorption in the crystal of olivine are obtained, respectively.
2. At micro scale (10μm) scale, the olivine micro scale transient saturated dislocations/defects propagation in coupled thermal-force-time fields is calculated, the relationship between the crack propagation-evolution, stress distribution and micro strain under different velocity and time conditions is obtained,

All these findings can helpful understand the mechanism of the dehydration fracturing shale gas, the coal-gas outbursts, and coseismic triggering problem.

PROSPECT AND FUTURE WORK

Multi temporal-spatial structure and performance relationship the fundamental issue in physics, material and mathematical fields in future years. So many complex and challenging multiple temporal-spatial unstable-stable evolutions problems included in geosciences field (earthquake and earth internal structure evolution) may be major breakthrough if above mechanism is cleared. Energy theory, different from the classical Newtonian mechanics and involved quantum mechanics, is one of the possible methods for solving above issue. Combined with ultra-high performance simulation and high developing experiment technology, as a revolution of mechanics/physics, the lowest level matter evolution micro-transient-mechanism may be found.

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