

Molecular dynamics simulation to reveal slip and lubrication behaviors of interfacial water on quartz at high temperature conditions

*Satoru Ishikawa¹, Hiroshi Sakuma², Noriyoshi Tsuchiya¹

1. Graduate School of Environmental Studies, Tohoku University, 2. National Institute for Materials Science

Water-rock interaction has many important roles in Earth's events such as earthquake. The relationship between fault friction and geofluid has been studied as represented by Sibson *et al.* (1988). The frictional strength of fault under the presence of fluid is controlled by phenomena occurring at the interfaces of mineral surface and fluids. Such interfaces can be understood from micro- and nano-scale approaches. The physicochemical properties of interfacial water on a solid surface have been studied by both theoretical and experimental methods. In our previous molecular dynamics study (Ishikawa *et al.*, 2016), interfacial water on quartz at 298-573 K showed layered structure and lower self-diffusion coefficient than that of bulk water. This indicates that, even at high temperature condition like underground environment, physicochemical properties of interfacial water on mineral could be different from bulk water. This interfacial water may alter the frictional strength of faults. In this study, we performed molecular dynamics simulations to understand the effects of interfacial water on the friction between quartz surfaces at 298-573K.

We prepared the system of confined water between two quartz surfaces characterized by the termination of silanol (Si-OH). The thickness of confined water layer ranges from 0.3 to 3 nm. In the simulation, surface force balance (SFB) system was used (Leng and Cummings, 2006). One quartz surface was fixed and the other surface was moving with constant velocity. The shear force of moving surface was calculated to obtain the friction coefficient.

In our presentation, we will show the lubrication behavior of interfacial water at 298-573 K and the discussion of frictional behavior on fault with pressurization.

Sibson *et al.* (1988) *Geology*

Ishikawa *et al.* (2016) *J. Mineral. Petrol. Sci.*

Leng and Cummings (2006) *J. Chem. Phys.*

Keywords: Molecular dynamics, interfacial water, friction

Molecular simulation of density fluctuation of H₂O and H₂O-NaCl solutions under supercritical conditions

*Satoru Ishikawa¹, Kazuma Sato¹, Nobuo Hirano¹, Noriyoshi Tsuchiya¹

1. Graduate School of Environmental Studies, Tohoku University

Supercritical fluids, which the density of the liquid phase and the vapor phase are equal, have characteristic properties on chemical reactivity, solubility, and ionic product. The fluids are under the condition higher temperature and higher pressure than the critical point. Geofluids, which is mainly composed in H₂O-NaCl are sometimes identified as supercritical state in deep areas such as earth's crust, deep-sea hydrothermal vents and deep-drilling for geothermal well. The physicochemical properties of supercritical geofluids are important to understand these areas.

Molecules of supercritical fluid are heterogeneously distributed, and forming density fluctuation. The characteristic properties of supercritical fluids are said to be mainly due to the density fluctuation. Direct observation on the density fluctuation is obtained by small-angle X-ray scattering (SAXS) (Nishikawa *et al.*, 1996) and visible light spectroscopy (Tsuchiya and Hirano, 2007; Sekiguchi *et al.*, 2013). On the other hand, molecular dynamics simulations of supercritical fluids have been performed focused on the molecular cluster size (Istok *et al.*, 2008). Here, we performed molecular dynamics simulations of H₂O system and H₂O-NaCl system at high temperature conditions around the critical point.

H₂O molecules and H₂O-NaCl molecules were prepared in a cubic box. In order to evaluate the density fluctuation, "bin analysis method" was used. This method divides the cubic box into small cubes with equal volumes, and the number of molecules in each boxes was counted at each time steps. The distribution of the number of molecules in each small boxes has a normal distribution and some amount of standard deviation. Large standard deviation means that the density fluctuation is large. As the result of the simulations, the density fluctuation of H₂O and H₂O-NaCl was maxima around the critical point. In our poster, we will show the behavior of NaCl concentration dependence, and discuss about the effect of Na⁺ and Cl⁻ ion.

Nishikawa K. and Tanaka I. (1996) *J. Phys Chem.*

Tsuchiya N. and Hirano N. (2007) *Island Arc*

Sekiguchi *et al.* (2013) *J. Mineral. Petrol. Sci.*

Istok *et al.* (2008) *J. Phys. Chem.*

Keywords: supercritical water, Molecular dynamics

Permeability evolution in high-temperature fractured granite by water-rock reaction at elastic and plastic conditions

*Kohei Saito¹, Noriaki Watanabe¹, Atsushi Okamoto¹

1. Graduate School of Environmental Studies, Tohoku University

A new and economically attractive type of geothermal resource was recently discovered in the Krafla volcanic system, Iceland, consisting of supercritical water at 450°C. Moreover, a recent study on permeability of fractured granite at temperatures exceeding the brittle-ductile transition (BDT) temperature of ca. 360°C has suggested that potentially exploitable supercritical geothermal resources may form even in the ductile granitic crust. This is because high permeability may be created by tensile fracturing such as hydraulic fracturing in the ductile crust, in which shear fracturing may not be likely, and the created permeability may not be destroyed even though a transition from elastic to plastic deformation of fracture surfaces (elastic-plastic transition) leads to strongly stress-dependent and irreversible permeability. However, there is still concern about viability of permeability because previous studies have suggested that fracture permeability reduction occurs with time at high temperature and high effective confining stress conditions due to pressure solution at bridging asperities within the fracture, and an increase of permeability reduction rate by the elastic-plastic transition is also suggested. In the present study, hydrothermal flow-through experiments have been conducted on granite samples containing a single tensile fracture at 400°C, a pore pressure of 10 MPa, and effective confining stresses of 18, 30 and 50 MPa, with a flow rate of 0.1 g/min, where the elastic-plastic transition stress at 400°C is 40 MPa. Permeability reduction was observed at 30 and 50 MPa, where the permeability reduction was faster for the higher stress level. On the other hand, permeability increased at 18 MPa. Permeability reduction rate was positively correlated with effective confining stress, as expected from the theory of pressure solution. However, the increase of the reduction rate from 30 MPa to 50 MPa (elastic to plastic conditions) was larger than that from 18 MPa to 30 MPa (elastic to elastic conditions). These results imply that dissolution was dominant reaction in these experiments, and permeability increased and decreased respectively at the lowest and other stress levels depending on influence of the pressure solution. Moreover, these results imply an acceleration of permeability reduction rate (i.e, pressure solution) by the elastic-plastic transition. The permeability reduction rate at the plastic condition seemed to be several times larger than that at the elastic condition.

Keywords: permeability, ductile crust, supercritical geothermal resource

Permeability enhancement of granite fracture followed by seismic slip in laboratory experiments

*Takuya ISHIBASHI¹, Hiroshi ASANUMA¹, Derek ELSWORTH², Yi FANG², Jacques RIVIERE², Chris MARONE²

1. Fukushima Renewable Energy Institute, National Institute of Advanced Industrial Science and Technology, 2. The Pennsylvania State University

Hydraulic stimulation for the fractured reservoirs such as geothermal and hydrocarbon reservoirs is now a well-known operation for enhancing or maintaining the permeability of reservoir [Evans *et al.*, 2005; Häring *et al.*, 2008]. In this operation, as a massive amount of pressurized fluid is injected into the targeted reservoir, preexistent fractures undergo slip/shearing. At the period of fracture slip/shearing, seismicity is triggered in both seismic and aseismic modes [Ellsworth, 2013]. Here, considering the fact that the crustal permeability is the essential factor for controlling the fluid flow in the Earth's crust [Ingebritsen and Manning, 2010] and the permeability change of rock fracture is closely related to the changes in pore pressure and effective normal stress of rock fracture, it is no wonder that we come to interest in the relationship among frictional strength evolution, fracture permeability evolution, and the manner of seismicity (i.e., seismic or aseismic) during slip/shearing. Although such a relation is fundamental for defining the impact of the hydraulic stimulation or for simulating the nucleation of seismicity adequately [McClure and Horne, 2012; Norbeck and Horne, 2016], this relation has rarely been investigated and is still poorly understood.

The present study explores this relationship via the laboratory shear-flow concurrent experiments on the Westerly granite fracture. The novelty of our experiment is the fact that the shear velocity is precisely controlled during the fracture permeability measurements. Experimental results demonstrate the possibility that the permeability enhancement of rock fracture is created by frictional shearing of velocity-weakening (potentially unstable slip). To proceed our discussions on this link, we further evaluate the state of contacting asperities and of fracture surface asperities via statistically equivalent digital rock fracture modeling. By combining the experimental study with the numerical study, we can first discuss the aforementioned relationship, and successfully propose the two plausible mechanisms constraining the relationship; change in contacts distribution and shear-induced dilation at the moment of the instantaneous shear velocity jump. Though we haven't completely specified the mechanism that indeed controls the link between mechanical and hydraulic properties of rock fracture herein, these mechanisms should be taken into account in interpreting the field observation such as the abrupt permeability increase of natural fault at the moment of seismic slips [e.g., Guglielmi *et al.*, 2015].

Keywords: fracture permeability, seismic slip, contacts asperities, frictional coefficient

Slip characteristic of rock fracture in brittle-ductile zone

*Sho Takeyama¹, Noriaki Watanabe¹, Kiyotoshi Sakaguchi¹, Noriyoshi Tsuchiya¹

1. Graduate School of Environmental Studies, Tohoku University

The geothermal energy using the fracture-type reservoir in the continent crust more than temperature of brittle-ductile transition (350 °C - 400 °C) is suggested. When using this fracture-type reservoir, there is a possibility of aseismic slip rather than seismic slip. However, characteristic and influence on permeability of the aseismic slip is unknown. Therefore, in this study, to clarify the occurrence condition, characteristics, influence on permeability of aseismic slip, injection-induced slip experiment using cylindrical specimen with 60 °tilted crack was conducted at elastic-plastic deformation condition. As a result, the slip behavior suggested the occurrence of aseismic slip under both conditions of elastic deformation condition and plastic deformation condition. The magnitude of slip under elastic deformation condition was bigger than that under plastic deformation condition. In addition, the penetration rate increased by 24 times under the elastic deformation condition and 2 times under the plastic deformation condition.

Keywords: Slip characteristic, brittle-ductile transition zone

Mechanical properties of granites after triaxial deformation and fracturing in hydrothermal conditions under supercritical state

*Manami Kitamura¹, Miki Takahashi¹, Kenta Takagi², Nobuo Hirano², Noriyoshi Tsuchiya²

1. National Institute of Advanced Industrial Science and Technology, 2. Graduate school of Environmental Studies, Tohoku University

In order to extract geothermal energy effectively and safely from magma and/or adjacent hot rock, we need to tackle many issues which require new technology development, such as a technique to control a risk from induced-earthquakes. On a development of induced-earthquake mitigation technology, it is required to comprehensively understand roles of factors on occurrences of the induced-earthquake (e.g., regional and local stress conditions, strength of the hot rock, pore pressure of supercritical fluid, crack density or porosity, permeability and fluid-rock reaction) and their intercorrelations (e.g., *Asanuma et al., 2012*).

Our purpose of this first series of the experiments is to clarify a relationship between the rock strength and the crack density under the supercritical fluid conditions. Although in this abstract we only show a preliminary result of triaxial deformation experiment on intact granite rock strength under high-temperature (250–650 °C), high-pressure (104 MPa) condition at a constant load-point velocity (0.1 μm/sec) using a gas-rig at GSJ/AIST, we at JpGU meeting will report alteration of the granite rock strength relevant to crack density increase. We used Oshima granite as the specimen for the deformation, which has initially less than 0.2 % of the porosity and 4.29 ± 0.55 km/s in V_p (dry) and 2.49 ± 0.19 km/s in V_s (dry), respectively. All experimental products showed the brittle feature having several oblique fracture surfaces with c.a. 35° to cylindrical axis of the specimen, but the amount of stress drop became smaller at higher temperature and/or at lower pore pressure. Estimated Young's modulus increased with decreasing the temperature from 35.9 GPa at 650 °C to 57.4 GPa at 250 °C. At 550 °C, the stress drop accelerated the deformation with 8~10 times faster velocity than that at load-point. In contrast, at 650 °C, the velocity during stress drop kept the velocity within the same order of the load-point velocity. Therefore, the deformation mechanism may start to be changed from brittle to ductile when the temperature exceeds 650 °C, even though the brittle fracture is observed.

Highly dense cracked granite specimens were formed by a rapid decompression treatment using an autoclave settled at Tohoku University (*Hirano et al., 2016 JpGU*), caused by a reduction of the fluid pressure within several seconds from vapor/supercritical state (10–48 MPa, 550 °C) to ambient pressure. X-ray CT scanning on the specimens after the rapid decompression treatment let us recognize that numerous microcracks developed mainly along grain boundaries. Using X-ray CT images, we also have a plan to evaluate the fracture density for the fractured granite rock specimens. The rapid decompression treatment imposed the porosity increasing towards 3.75 % and V_p and V_s decreasing towards 1.37 ± 0.52 km/s and 0.97 ± 0.25 km/s on the specimens, respectively. In future, we will compare the strength for the intact granite rocks resulted from the triaxial deformation experiments with that for the fractured granite rocks to create the relationship between the granite strength and the fracture density under the supercritical conditions.

Keywords: Supercritical geothermal resources, Rapid decompression fracturing, Brittle-ductile transition zone, Granite

Real-time measurements of permeability of Aji granite during triaxial compression tests

*Sueyoshi Kazumasa¹, Ikuo Katayama¹

1. Department of Earth and Planetary Systems Science, Hiroshima University

Hot dry rock power generation, one kind of the geothermal generation, is a generation system which uses technique to create an artificial geothermal fluid reservoir by the hydraulic fracturing of bedrock. This generation system is expected to generate more electricity compared with conventional geothermal generation because it can develop a much wider range of sites. In the reservoir, water transportation is restricted by the permeability of host rock (Townend and Zoback, 2000). Therefore, it is important to know how the permeability varies with deformation of host rock. Permeability variations in the process of deformation of granite have presented by Zoback and Byerlee (1975) and Mitchell and Faulkner (2008). However, there are some problems in their studies. First, permeability of prefailure sample was not measured. Second, their results of measurements are not continuous. Third, their results lack accuracy. This study aims to improve these problems and measure permeability in the process of granite deformation during triaxial compression tests.

Aji granite which was formed into cylindrical shape (20 mm long and 40 mm in diameter) was used as a specimen and a nitrogen gas was used as the pore fluid. The triaxial compression tests were conducted with Intra-Vessel Deformation and Fluid-Flow Apparatus (IVA) at constant pore pressure (1.5MPa), confining pressure (20 or 40MPa), displacement rate (0.02 or 0.04mm/min) and room temperature. All the experiments were performed by using a flow method and the permeability was calculated from the flow rate which was measured in every ten seconds. In addition, strain measurements by a strain gauge were performed at the same time. The relationship between the permeability and inelastic volumetric strain was investigated.

The experimental results showed that the permeability initially decreased and began to increase from the onset of dilatancy. Regardless of the experimental condition, variation of the permeability had this tendency. This indicates that as the sample initially stressed, preexisting cracks closed and new cracks were created by inelastic deformation with increasing differential stress. The permeability increased along with inelastic volumetric strain. As samples approached brittle failure, the permeability increased remarkably. The previous research reported that mean crack diameter increased in the prefailure stage (Takemura and Oda, 2004). Therefore, the permeability enhancement in the prefailure stage is due to the increase in crack diameter.

Keywords: Permeability, Dilatancy, Inelastic volumetric strain

Fundamental study of flush fracturing of high temperature controlled by depressure rate

*Kenta Takagi¹, Hirano Nobuo¹, Noriyoshi Tsuchiya¹

1. Graduate School of Environmental Studies, Tohoku University

Generating cracks to rock can be applied to deep drilling technology for seated geothermal development. Thermal stress derived from rapid decompression is considered to be effective for crack generation of rocks. But possible bottomhole decompression condition is milder than that of previous studies. In this study, rapid decompression experiment at 500, 550 and 600 °C for granite samples with water/rock ratio of 2.5, 0.5 and 0.2 was conducted. And after experiment porosity and P-wave velocity (V_p) were measured. As temperature and water/rock ratio increase, the temperature after decompression was decreased (ΔT as temperature difference of before/after decompression was increase.). Porosity is largely depending on temperature before decompression, in particular a-b phase transition of quartz has large influence. V_p is also depends on temperature before decompression. And V_p of sample at 600 °C decompression has same as water. Differences of water-saturated V_p and dry condition V_p shows the relationship of ΔT . Therefore ΔT affects the process of crack generation. When ΔT is small, micro crack is generated, and when ΔT is large, large aperture crack is generated. Elastic moduli were calculated from porosity and V_p . Young's modulus decreases as porosity increases and shows negative value in all after decompression samples, which indicates samples after decompression are no more elastic. This result shows that it is possible to generate small cracks to rock even if ΔT is small.

Evaluation of Deep Geothermal Reservoir and Magma Process Revealed by Melt Inclusion-Example in Fukano Caldera, NE Japan-

*Fajar Febiani Amanda¹, Ryoichi Yamada¹, Masaoki Uno¹, Noriyoshi Tsuchiya¹

1. Graduate School of Environmental Studies, Tohoku University

INTRODUCTION

The deep geothermal reservoir which located beneath the caldera is potential energy resources. Magma process and the formation of the caldera were important geological evidence to reveal deep-seated geothermal reservoir, and caldera fill sediments provide petrological evidence of volcanic activities. Melt inclusion is a reliable material that provides the thermal-chemical information of the magma chamber, as it preserves the composition of the magma before eruptions. This characteristic has been used by the petrologists to determine magma evolution and differentiation. In this study, melt inclusion is used to evaluate the properties of geothermal resources, including the depth, and differentiation process which were conduct in Fukano Caldera Northeast Japan.

Fukano caldera located in the West of Sendai City. This caldera activity started from 7-8 Ma based on stratigraphy and the fossil data (Otsuki et al. 1995). Fukano formation filled in Fukano Caldera is characterized by whitish to grayish white colored massive pyroclastic flow deposits which are composed of small amounts of pumice and volcanic lapilli with 10 to 20 mm in diameter. Tenjin tuff member is grayish white massive pumiceous pyroclastic flow deposit which is contained huge dark colored pumice blocks (size up to 30 cm) and also is intercalated with lake sediments (Takahashi & Nagahashi, 2004).

METHODS

Samples were taken from 20 locations that represent the products of Fukano caldera (Fukano Formation & Tenjin Tuff member). These samples can be categorized into welded tuff and pumice tuff. Quartz crystals were separated from the samples, which are then encased with resin plate. The melt inclusions in quartz crystals are then analyzed using electron probe micro analyzer (EPMA) for 10 elements. The depth of crystallization is determined by the percentage of Quartz (Qtz) –Albite (Ab) –Orthoclase (Or) that calculated from CIPW norm. The eutectic lines will be shifted with the pressure so that if the composition of the melt inclusions in quartz crystals plotted on the diagram, quartz crystallization pressure can be calculated, as well as the emplacement depth. The MI sample then analyzed using LA-ICP-MS for 44 elements. The incompatible elements were normalized with basaltic andesite from the nearby recent volcanic arc (Zao Volcano, Tatsumi et al. 2008) to determine the differentiation of the magma.

ANALYSIS AND RESULT

The samples from Fukano Caldera were classified into low-medium K, low alkali tholeiite dacite-rhyolite with the higher silica content in the sample from the northern part. The norm percentage, crystallization pressure, and depth for the northern part and southern part respectively of 126 melt inclusions are Qtz: 20-46%, Ab: 44-71%, Or: 5-13%, 11-1900 MPa, 0.4-200km and Qtz: 29-41%, Ab: 55-66%, Or: 3.5-8%, 76-660 MPa, 3-24 km. The samples are following plagioclase differentiation path.

PRELIMINARY RESULT OF PETROCHEMICAL COMPARISON OF GRANITOIDS OF THE MANDAKH AREA IN SOUTH MONGOLIA

*Undarmaa Batsaikhan¹, Munkhtsengel Baatar², Batkhishig Bayaraa², Burenjargal Ulziiburen², Noriyoshi Tsuchiya¹

1. Graduate School of Environmental Studies, Tohoku University, 2. School of Geology and Mining Engineering, Mongolian University of Science and Technology

The Mandakh granitoids in southern Mongolia is part of the Central Asian Orogenic Belt, a vast accretionary orogen that records the opening and closer of the Paleo-Asian Ocean in the late Proterozoic to Palaeozoic. Our research area is located in Mankdakh soum of Dornogovi province in the southeast Mongolia. In the around Mandakh area, several granitoids, such as the Narin khudag, the Bronze fox, the Mandakh, the Mogoit, the Budar and the Shuteen, show different age several from early Carboniferous to Permian.

The previous researchers have studied some intrusive bodies, for example the Narin khudag, the Bronze fox, the Mandakh (James H.S.Blight et al., 2010), Shuteen (Batkhishig, Iizumi, 2001). However, no detailed analyses of other granitoid complexes have been carried out, therefore, we studied petrochemical properties of granitoids (Bronze fox (ca. 10 km²), the Budar (ca. 42 km²), the Mandakh (length stretched around 45 km), the Mogoit (ca. 40 km²)). The Harmagtai-Hongoot-Oyut and Tsagaan suvarga Cu-Mo porphyry ore bodies which were identified are distributed in and around the area as Middle Carboniferous to Early Permian and late-Devonian respectively.

The Mandakh complex contains porphyritic structure granite and granodiorite but the Mogoit and The Bronze fox intrusions composed from granite and quartzmonzonite, have medium (5-10mm) and coarse (>10mm) grained textures, that vary from equigranular to crystal-crowded porphyritic. The samples collected from the Bronze fox, the Budar, the Mandakh, the Mogoit complexes consist of ca 3-5 mm- long euhedral plagioclase phenocrysts that are strongly altered to sericite. The groundmass contains 2-3 mm biotites and interstitial quartz. Additionally, a medium-grained granitoid densely packed with subhedral 3-5 mm K-feldspar phenocrysts, which have an apparently poikilitic and perthitic texture. Accessory minerals include apatite, sphene and zircon. Intrusive rocks are immersed by K alteration and sericite-chlorite alteration assemblages.

The complexes of Mandakh area composed from high calc-alkaline, I-type. Furthermore those plutons are silica saturated SiO₂ 66 %, high Al₂O₃ 14.4 %, Na₂O+K₂O>6 %, Y25 ppm, Nb 12.3 ppm, Rb 150.1 ppm, formed within an island arc setting.

Porphyry Cu-Mo deposits and occurrences are associated with typical calc-alkaline metaluminous, oxidized, I type, magnetite series granitoids, which is dominated granitoid type in Mongolia (Gerel. O., et al). The petrochemical figure of granitoids of the Mandakh area is commonly similar to the Carboniferous Shuteen Complex which is petrochemically similar to adakite-type rocks.

Keywords: Mongolia, granitoid of Mandakh, Central Asian Orogenic Belt

Formation of mineralized quartz veins induced by flash evaporation from liquid to vapor under sub and supercritical conditions

*Takashi Amagai¹, Atsushi Okamoto¹, Noriyoshi Tsuchiya¹, Nobuo Hirano¹

1. Graduate school of environmental studies, Tohoku university

Fluid flow through faults and fractures in Earth's crust controls transport of elements, energy and heat, and it is associated with formation of many types of ore deposits. Since the solubility of silica in water drastically changes with temperature and pressure conditions, fluid flow and phase transition of aqueous fluids produce silica scales in pipelines of geothermal power plants and also mineralized quartz veins. A drop of fluid pressure and involving boiling could be a cause of precipitation of silica and metal species. Weatherley and Henley (2013) proposed a hypothesis of gold mineralization by "flash vaporization", which is an instantaneous vaporization at fault jog induced by fault displacement. They suggested a possibility of the formation of gold-quartz veins at the time of earthquake. Since there are many similarities between conditions of supercritical geothermal reservoir and hydrothermal ore deposits, the exploitation of supercritical geothermal reservoirs would provide us good opportunities for further understanding mechanism of hydrothermal ore deposits. However, to our knowledge, there have been no studies on precipitation of silica under such extremely high-supersaturated conditions, and its relation to ore formation. The aim of this study is to understand the mechanism of silica precipitation by flash vaporization and its relation to hydrothermal ore deposits. The reaction vessel (50 or 110 ml) has inner wall made of Ti, and P-T conditions were up to 450 and 50 MPa, respectively. Initially, we enclosed the fluids into the vessel, elevated pressure and temperature, and then, flashed fluids by opening the valve. Alumina filter with pore size of 10-30 micron was placed on the flow path to catch precipitates during vaporization.

In the experiments of silica precipitation by flashing, the input solution (Si = 370 ppm) was prepared by dissolution of composites of quartz and granite sand. The rapid decompression experiment was carried out by flashing from 30 MPa under liquid (200, 250, 300, 350°C) and supercritical conditions (400, 450°C). The pressure of the input solution was instantaneously decrease to the vapor conditions within a few seconds. In contrast to our previous studies of silica precipitation by flow-through apparatus (Okamoto et al. 2010), where phase transition of water occurred by increasing temperature, silica precipitates did not include quartz but occurred as spherical particles of amorphous silica with size of 1-3 micron, probably due to a lack of duration of transformation into more stable phases. The Si concentration of the output solution ranged from 10 to 60 ppm, which is lower than the solubility of silica on the saturated vapor pressure curve along the P-T path. These occurrences of silica indicate that metastable amorphous silica particles were formed by rapid decompression and transported from sub- to supercritical fluids, which leads to the formation of silica scales and clogs of fractures.

Next, we prepared the initial fluids (pH = 2, HCl added) with metal components, Cu (170 ppm) and Mo (30ppm), as well as silica (Si = 400 ppm). The input solution was kept four hours at 350°C, 30 MPa, then was decompressed in two ways; first one is slow decompression by natural cooling, and the other was near adiabatic decompression by flash vaporization. As the result of slow decompression, the composition of the solution after the experiment does not change significantly (Si = 360 ppm, Cu = 130 ppm, Mo = 12 ppm). In contrast, in the rapid decompression experiment, each concentration decreased drastically to Si = 13 ppm, Cu = 4 ppm, Mo = 0.2 ppm, respectively. Our results indicate that mechanism and rate of the formation of mineralized quartz veins was highly depends of P-T-t path of the fluids, and that flashing from

sub to supercritical conditions (phase transition of water) potentially plays roles of mineralization.

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Keywords: Flash vaporization, Supercritical fluid, Quartz vein