

**Phase equilibria modeling of anatexis during ultra-high temperature
metamorphism of the crust**

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ABSTRACT

Ultra-high temperature (UHT) granulite-facies metamorphism is commonly identified in Mg–Al-rich rocks. Many such lithologies are thought to be metasedimentary rocks based on the presence of detrital zircon. However, whether a metasedimentary protolith is required to form diagnostic mineral assemblages and how much melt is lost during burial and heating to reach UHT conditions varies significantly according to the prograde pressure–temperature path. In this study, integrated thermodynamic modeling, accessory mineral modeling, and trace element modeling has been conducted on an average metapelite composition and average mid-ocean ridge basalt (MORB) composition under open-system conditions. The results show at least three and two melt loss events occur before reaching UHT conditions in initially water-saturated pelitic and basaltic rocks, respectively. Around 22–27 vol. % S-type granite and 12–17 vol. % I-type granite would be produced during these evolutions, respectively. For pre-conditioned (dry) protoliths, however, melt loss is not required to reach UHT conditions. Melt extraction leads to an increase of Al and Mg in metapelite residua. Given a relatively Mg-rich protolith, mineral assemblage sapphirine + quartz is then allowed to form at higher grades; however, metabasalt does not form these UHT diagnostic assemblages, regardless of the amount of melt lost. During equilibrium melting, crustal differentiation induced by UHT metamorphism would significantly reduce the amount of heat-producing elements (HPEs) in the melt-depleted residuum, which progressively decreases a rock’s heat production capacity. In reality, however, new monazite grains likely form during peak metamorphism and some monazite grains would be shielded by porphyroblasts, resulting in an increase of Th in the residua during heating. Even so, we suggest the efficiency of heat production would still decrease, given the heat production rate of Th is much lower than U. Considering some granitic rocks with relatively high heat production are

35 emplaced into the granulite terrane, we suggest that radioactive heat production may be a
36 contributing driving force for UHT metamorphism; however, it is not sufficient. Most heat
37 required to generate UHT granulites must come from hybrid sources, such as advected heat from
38 the mantle, conducted heat from nearby magmatic intrusions, radioactive heat production, and
39 exothermic mineral reactions.

40 **Key words:** anatexis; crustal differentiation; forward modeling; open system; ultra-high
41 temperature

1 INTRODUCTION

Ultra-high temperature (UHT) metamorphism ($>900\text{ }^{\circ}\text{C}$ at $0.7\text{--}1.3\text{ GPa}$) is the most thermally extreme condition that the continental crust may achieve (Harley, 1998, 2008), and several UHT localities have been identified throughout the geological record in rocks of Archean to Miocene age (Kelsey, 2008; Kelsey & Hand, 2015). Most UHT granulites have been recognized based on the diagnostic parageneses sapphirine + quartz, high-Al orthopyroxene + sillimanite, and osumilite-bearing mineral assemblages, which only stabilize in Mg–Al-rich bulk compositions; however, Mg–Al-rich granulites are volumetrically scarce in nature and have no geochemically equivalent sedimentary or igneous protolith (Chinner & Sweatman, 1968), making their origin controversial. Based on detrital zircon evidence and field relationships, Kelsey & Hand (2015) concluded that the most likely candidates were sedimentary rocks that had experienced significant partial melting (e.g. Drüppel, Elsäßer, Brandt, & Gerdes, 2013; Ellis, 1980; Reinhardt, 1987; Sheraton, 1980; Sheraton, Tingey, Black, Offe, & Ellis, 1987), although this hypothesis has yet to be rigorously tested.

Crustal melting (anatexis) is ubiquitous in the middle and lower crust and plays an important role in crustal reworking and intracrustal differentiation (Sawyer, Cesare, & Brown, 2011). Anatexis is a key process that generates voluminous granitic melt that forms a major component of Earth's upper continental crust, and melting may be induced by magmatic underplating, lithospheric extension, upwelling of asthenosphere, or an elevated concentration of heat-producing elements (Andreoli, Hart, Ashwal, & Coetzee, 2006; Clark, Fitzsimons, Healy, & Harley, 2011; Dewey, Robb, & Van Schalkwyk, 2006; McLaren, Sandiford, Powell, Neumann, & Woodhead, 2006; Yakymchuk, 2019).

If crustal anatexis and/or intracrustal differentiation is required to form Mg–Al-rich rocks that may then be metamorphosed and form UHT mineral assemblages (Baba, 2003; Brandt, Will, & Klemm, 2007; Clifford, Stumpfl, Burger, McCarthy, & Rex, 1981; Droop & Bucher-Nurminen, 1984; Lal, Ackermann, Seifert, & Haldar, 1978; Raith, Karmakar, & Brown, 1997), systematic analysis of the fertility of likely precursor rocks should be able to identify the formation of these rare, but important, granulites, and also to provide key information about granite generation and the heat budget of the middle to lower crust. In this study, we briefly introduce the tectonic scenarios that can generate UHT metamorphism and their associated pressure–temperature (P – T) paths. Second, we use petrological forward modeling to quantify the amount of melt extraction required to generate UHT granulites along with the changing chemical composition of the melt and residua in each tectonic setting. These results are then coupled with geochemical trace element analysis and estimation of the heat budget of each lithology. These modeling results thus provide new understandings of the relationship between UHT metamorphism and crustal anatexis.

2 TECTONIC ENVIRONMENTS CONDUCTIVE FOR UHT METAMORPHISM

From an energetic point of view, heat produced in the lithosphere is redistributed by conduction and advection (Stüwe, 2007). Given the slow rates of thermal diffusion in silicate rocks, UHT metamorphism is difficult to induce purely via conductive heat transfer (Brown, 2008; Jaeger, 1964; Sandiford & Hand, 1998; Stüwe, 2007; Whittington, Hofmeister, & Nabelek, 2009). As such, several possible alternative heat sources have been proposed for raising the temperature of the crust at a regional scale, including advected heat from mafic magmatic intrusion, elevated concentrations of heat-producing elements coupled with slow erosion, and

ductile shearing (e.g. Clark *et al.*, 2011; Huang, Guo, Jiao, & Palin, 2019; Nabelek, Whittington, & Hofmeister, 2010; Vielzeuf, Clemens, Pin, & Minet, 1990).

Since melting is an endothermic process that buffers temperature increase (Stüwe, 1995), anatectic reactions will proceed until a reactant mineral is totally consumed, after which a rock may continue to heat up (Clemens, 2012; Schorn, Diener, Powell & Stüwe, 2018; Schorn & Diener, 2019). In such case, a previous episode of metamorphism may precondition the crust to allow it to reach the UHT condition. Beyond that, only a strong thermal anomaly combined with efficient melt extraction can drive rocks toward UHT conditions at a regional scale (Clark *et al.*, 2011; Clemens, 2012). Several possible tectonic scenarios for generating UHT metamorphism can then be defined, including:

Melt-bearing mantle upwellings or underplating of mafic magma beneath a continental arc. This model has been proposed to explain extensive exposures of UHT granulites in Precambrian terranes. Owing to higher mantle potential temperatures during the Archean compared to today (Herzberg, Condie, & Korenaga, 2010), a weaker crust-mantle coupling on the early Earth would induce slab breakoff of subducted oceanic lithosphere at relatively shallow depths, followed by melt-bearing mantle upwelling and syn-rifting magmatic underplating. Rocks at the base of the overriding plate would then experience isobaric heating to UHT conditions (Sizova, Gerya, & Brown, 2014), as is noted from many Archean terranes worldwide. This model is broadly similar with ridge subduction and the back-arc model suggested by several researchers to explain some Phanerozoic UHT terranes (Kemp, Shimura, Hawkesworth, & EIMF, 2007; Pownall, Hall, Armstrong, & Forster, 2014).

Orogen self-heating. Owing to the paucity of basic intrusions in many UHT terranes, Clark *et al.* (2011) proposed an orogenic self-heating model to explain long-duration and extensive UHT

metamorphism. In this model, a long-lived overthickened hinterland with abundant heat-producing elements and low erosion rate would generate UHT granulites without any advective heat from magmatism. Rocks in this model would most likely experience heating during burial to peak pressure conditions, followed by decompression and heating to reach UHT conditions.

Multi-period thermal anomaly. Most granulites have experienced more than one period of heating (e.g. Kelsey & Hand, 2015). In some cases, they would experience a prolonged metamorphism, during which discrete episodes would sequentially heat up the granulite during residence in the lower crust. For example, metamorphic zircon in UHT granulites from the Khondalite Belt, North China Craton, record a continuous age range of formation from *c.* 1.96 to *c.* 1.88 Ga, with peaks at 1.95 Ga and 1.92 Ga (Huang *et al.*, 2019). Here, the older peak age of *c.* 1.95 Ga is interpreted as a precursor granulite-facies metamorphism event driven by the collision between two Archean blocks, leaving a pre-conditioned (dry) residual source rock that was then exhumed to the middle crust. Later mantle-derived mafic magmatism then heated the residual granulites to UHT conditions at *c.* 1.92 Ga. These rocks thus experienced a continuous *P–T* path showing compression and heating processes during prograde metamorphism, pseudo-isothermal decompression to shallower depths, and then isobaric second-stage heating to UHT conditions. In other cases, UHT granulites might experience polymetamorphism, which would not have a characteristic and continuous *P–T* path. We would not propose a possible *P–T* path in such case, but acknowledge the existence of this tectonic scenario. Nonetheless, it is important that all three of these tectonic scenarios are characterized by different *P–T* paths, which allow examination of the petrological evolution of different protoliths to be examined independently.

3 METHODS

3.1 Determination of initial bulk rock composition for modeling

When considering potential bulk-rock compositions for petrological modeling, it is key to consider the volume of melt that may be generated and lost from each lithology. Most crustal rocks may melt at temperatures as low as 650 °C in the presence of free H₂O-rich fluid (Brown, 2007; Palin and Dyck, 2020); however, fluid-present melting reactions have negative dP/dT slopes and are accompanied by a bulk volume reduction, limiting the amount of melt that can form and escape from the local environment (Clemens & Droop, 1998). Upon consumption of all free fluid, hydrous minerals, such as muscovite and biotite in meta-sedimentary rocks, and hornblende in meta-basic rocks, may progressively break down to generate melt and peritectic anhydrous minerals (Palin *et al.*, 2016, White & Powell, 2002). Owing to positive dP/dT slopes and a net increase in volume over the course of each reaction, large amounts of melt can be generated by fluid-absent anatexis, and so escape once a critical threshold is breached (Clemens & Droop, 1998). Such processes are thought to be the primary mechanism for crustal differentiation (Brown, 2013; Clemens, 2012; Sawyer *et al.*, 2011; Yakymchuk, 2019). All micas are typically consumed upon reaching UHT conditions, and if most of the melt has already drained away, the fertility of the residuum is significantly reduced and the composition of any new melt produced via anhydrous mineral breakdown is no longer granitic (Sawyer *et al.*, 2011).

Based on this model, two bulk rock compositions were selected for phase equilibria modeling: an average amphibolite-facies pelite (Ague, 1991) and an average mid-ocean ridge basalt (MORB) glass (Albarède, 2005). The initial H₂O contents in each were adjusted so that minimal (<0.1 mol. %) free H₂O occurred at the intersect of solidus and each P – T path, which applies a fluid-absent condition above the solidus (White, 2003; White, Pomroy, & Powell,

2005; White & Powell, 2002; Yakymchuk & Brown, 2014a, 2019; Yachymchuk, Kirkland, & Clark, 2018). This ensures that melt formation is not overestimated during early anatexis. The maximum melt proportion generated before drainage occurs – the melt connectivity transition (MCT) – was taken to be 7 vol. % for both lithologies (Rosenberg & Handy, 2005). Here, 6 vol. % was removed in each melt loss event (MLE) to simulate the common observation of small proportions (~1 vol. %) remaining on grain boundaries in rapidly chilled and drained migmatites (Yakymchuk & Brown, 2014a).

3.2 P – T paths selection

Three P – T paths were used for phase equilibria modeling based on the possible tectonic scenarios for UHT metamorphism described above. P – T path 1 involves isobaric heating at 0.8 GPa, corresponding to a melt-bearing mantle upwelling or basic magma underplating at a convergent continental margin (Sizova *et al.*, 2014). The pressure of 0.8 GPa was chosen to represent rocks in the lower crust of extensional tectonic settings, and so are located close to the onset of UHT metamorphism as defined in P – T space. P – T path 2 represents the orogen self-heating model (Clark *et al.*, 2011), comprising compression-heating from 0.75 GPa at the solidus to 1.5 GPa at 850 °C followed by decompression-heating to 0.75 GPa at 1000 °C. The geothermal gradient of the peak condition (567 °C/GPa) represents typical intermediate dT/dP type metamorphism, representing high-pressure granulite (Brown & Johnson, 2018). P – T path 3 represents a multi-period thermal anomaly model (Huang *et al.*, 2019). This P – T path follows the same prograde evolution as P – T path 2 up to peak pressure of 1.5 GPa at 850 °C, followed by isothermal decompression to 0.75 GPa at 850 °C, and a final period of heating to 1000 °C at 0.75 GPa.

3.3 Phase equilibria modeling

Phase diagrams were calculated using THERMOCALC v. 3.40 (Powell & Holland, 1988) and the internally consistent data set (ds62) of Holland & Powell (2011). Both pelitic and basaltic bulk rock compositions were modeled in the $\text{Na}_2\text{O}-\text{CaO}-\text{K}_2\text{O}-\text{FeO}-\text{MgO}-\text{Al}_2\text{O}_3-\text{SiO}_2-\text{H}_2\text{O}-\text{TiO}_2-\text{O}_2$ (NCKFMASHTO) chemical system. Activity–composition ($a-x$) relations used for pelitic compositions were taken from White, Powell, Holland, Johnson, & Green (2014), and those for basaltic compositions comprised clinoamphibole, augite, and metabasite melt (Green *et al.*, 2016), orthopyroxene, garnet and biotite (White *et al.*, 2014), plagioclase and K-feldspar (Holland & Powell, 2003), ilmenite (White, Powell, Holland, & Worley, 2000) and magnetite (White, Powell, & Clarke, 2002). Quartz and rutile were considered as pure phases. Removal of six-sevenths of the melt present where each P – T path intersects the 7 mol. % melt isopleth was conducted by manipulating ‘rbi’ script in THERMOCALC, as described in Yakymchuk & Brown (2014a). The bulk compositions used for phase equilibria modeling and the compositions of extracted melt are listed in Table S1–2. The densities of the residua were calculated by using the ‘calc sv’ script in THERMOCALC.

3.4 Trace element modeling

Trace element modeling was carried out using the batch melting equation $C_{\text{melt}}/C_{\text{source}} = 1/[D + F \times (1 - D)]$ (Shaw, 1970), where C_{source} and C_{melt} represent concentrations of a trace element in the source rock and the resultant melt, respectively; $D (= \sum K_d \times X)$ is the bulk partition coefficient, where K_d is mineral/melt partition coefficient and X is mol. % of the mineral; and F is the degree of melting. Initial bulk concentrations of 0.19 wt. % P_2O_5 , 3.5 ppm U, 14 ppm Th, 150 ppm Zr, and 150 ppm LREE were used for the metapelite (Ague, 1991; Yakymchuk *et al.*, 2018), and 0.18 wt. % P_2O_5 , 0.138 ppm U, 2.83 ppm Th, and 118 ppm Zr

were used for MORB (Albarède, 2005). The proportions of accessory minerals were calculated using the refined zircon solubility model from Boehnke, Watson, Trail, Harrison, & Schmitt (2013), the monazite solubility model from Stepanov, Hermann, Rubatto, & Rapp (2012), and the apatite solubility model from Harrison & Watson (1984). Values for K_d were taken from Bédard (2006) and Yakymchuk *et al.* (2018). The amounts of accessory minerals retained in the residuals are listed in Table S3, and the calculated U and Th concentrations in residua are listed in Table S4.

4 PATH 1 – ISOBARIC HEATING AT 0.8 GPA

4.1 Closed system

Closed-system pseudosections for pelite and MORB bulk compositions are shown in Figure 1 and Figure 2, respectively, and molar proportion of solid and melt phases along this isobaric heating segment are shown on temperature-phase proportion diagrams (“modeboxes”) below the P – T diagrams.

For the metapelite, the closed-system phase diagram resembles that presented by Yakymchuk *et al.* (2018) and predicts that the rock experiences muscovite dehydration melting from the solidus up to 739 °C, producing 8 mol. % melt alongside peritectic K-feldspar via the reaction of $Ms + Qz \rightarrow Kfs + Al_2SiO_5 + \text{melt}$. Biotite content remains fixed at 27–28 mol. % at this stage. After muscovite is totally consumed, biotite starts to break down at 738–860 °C and generates up to 35 mol. % melt. The rate of melt production is low at the beginning of biotite consumption, but increases significantly after peritectic garnet stabilizes at 785 °C, marking the onset of the reaction of $Bt + Sill + Qz \rightarrow Grt + Kfs + \text{melt}$. After all hydrous minerals are consumed, anhydrous felsic minerals break down to generate melt. In this closed-system

environment, up to 70 mol. % of cumulative melt would be produced at 1000 °C. Notably, the diagnostic UHT mineral assemblage of Spr + Qz is not predicted, whereas Opx + Sil is predicted to occur at 1000–1020 °C. The calculated system density decreases continuously from 2.87 g/cm³ at subsolidus conditions to 2.68 g/cm³ at UHT conditions, corresponding to an volume increase during fluid absent melting (Clemens & Droop, 1998).

For metabasalt, the modeled P – T path does not allow garnet to stabilize in this MnO-absent compositional system, although natural metabasites contain small amounts of MnO that should expand garnet’s calculated stability slightly on the phase diagrams shown here. Nonetheless, the mineralogy and topology of the phase diagram is relatively simpler than those for the metapelite, owing to MORB’s lower SiO₂ and K₂O, leading to higher variance equilibria forming (Miyashiro, 1994; Huang, Brown, Guo, Piccoli, & Zhang, 2018). Anatexis begins at 660 °C upon consumption of hornblende and quartz, corresponding to the reaction $\text{Hbl} \pm \text{Qz} \rightarrow \text{Aug} + \text{Pl} + \text{melt}$. Orthopyroxene becomes stable at 855 °C, defining the beginning of granulite-facies metamorphism. At this point, 10 mol. % of cumulative melt would be generated. After that, hornblende breakdown would generate up to 35 mol. % of cumulative melt at 1000 °C. In this model, hornblende would remain stable up to at least 1000 °C, although in nature this is unlikely and may be a consequence of uncertainty in Al–Si partitioning between clinopyroxene and hornblende in the Green *et al.* (2016) a – x relation (cf. Forshaw, Waters, Pattison, Palin, & Gopon, 2019). Akin to the metapelite, the density of this closed system decreases continuously from subsolidus to UHT conditions, ranging between 3.04 and 2.89 g/cm³.

4.2 Open system

4.2.1 Phase diagrams

If melt can leave the local system when it reaches the MCT, bulk compositions must be continuously altered during metamorphism and melt loss. Here, pseudosection panels representing initial protolith composition and a sequence of progressively more residual bulk chemical compositions following MLEs are shown, and modebox diagrams are shown below each P – T diagram.

For the metapelite, five MLEs produce six pseudosection panels along the isobaric heating path at 0.8 GPa, as shown in Figure 3. The lowest-temperature panel matches the low-temperature portion of the pseudosection in Figure 1 and the temperature of the ‘seam’ between panels represents the condition of the first MLE. In this open-system environment, MLE 1 occurs during muscovite dehydration melting at 738 °C, and MLEs 2–5 occur due to biotite dehydration melting at 800 °C, 823 °C, 843 °C and 863 °C. At 1000 °C, the rock has lost ~27 mol. % of cumulative melt, which is clearly much less than the 70 mol. % cumulative melt predicted for a closed-system environment. Interestingly, Spr + Qz would form at 1038 °C at 0.8 GPa in this open system, whereas Opx + Sil is not predicted. The density of the system shows a smooth decrease in each pseudosection panel, but an overall step-increase from 2.87 to 3.00 g/cm³ over the course of the metamorphic event.

For open system melting of metabasalt (Figure 4), four MLEs are predicted at 829 °C, 864 °C, 924 °C, and 977 °C. When compared with a closed system scenario, the modeled isobaric heating to 1000 °C at 0.8 GPa would produce 22 mol. % of extracted melt, which is less than the closed system simulation (35 mol. %). In this open-system environment, orthopyroxene first stabilizes at 853 °C, which is almost identical to the closed system. This is likely a result of only one set of melt having been lost at that point, and so the bulk-rock compositions in both

cases remained fairly similar. Again, as seen in the metapelite, the density of the system shows a smooth decrease between MLEs, but an overall step-increase from 3.04 to 3.08 g/cm³.

4.2.2 Melt and residuum compositions

Changes in the major oxide compositions of both protoliths along the modeled isobaric heating P – T paths at 0.8 GPa calculated by THERMOCALC are shown in Figs. 5–8. Equivalent compositions along other proposed P – T paths described below are also compiled in these diagrams and Table S1–2 for ease of comparison. Figures 5 and 6 show the bulk compositions of the metapelite used in P – T diagrams modeling and extracted melts, respectively. Figures 7 and 8 present the bulk composition of the metabasalt and extracted melts, respectively. As a result of mass balance, extraction of melt that is depleted in any given component compared to the source will lead to an enrichment of the source, and vice versa (Rapp, Ryerson, & Miller, 1987). For the residua produced during metapelite anatexis, H₂O, SiO₂, K₂O, and Na₂O show step-like decreases, whereas Al₂O₃, CaO, MgO, FeO_t and TiO₂ show increases. Associated melt extracted from the system becomes progressively depleted in H₂O and Na₂O, but increases in SiO₂, Al₂O₃, CaO, MgO, and K₂O. FeO_t show an overall increase during metamorphism, but a slight decrease in the final extracted melt. For the metabasalt residuum, H₂O, SiO₂, K₂O, and Na₂O show step-like decreases up-grade, whereas CaO, MgO, and TiO₂ increase. Al₂O₃ and FeO_t are more complicated in their fine detail, but show an overall increase within the temperature interval of interest. Melt progressively lost from the system shows a progressive decrease in H₂O, SiO₂ and K₂O, but increase in CaO, MgO and FeO_t. Al₂O₃ and Na₂O contents remain more or less constant. Calculated changes in trace element (U and Th) concentrations in the metapelite and metabasalt residua through five and four melt loss events are shown in Figure 9 and Figure 10, respectively. For the metapelite, U shows a step-like decrease, whereas Th shows a slight

increase after the first two MLEs, and then drops off to very low concentrations. For the metabasalt, U and Th contents both decrease during heating to 1000 °C.

4.2.3 Heat production values

The capacity for heat production within the residuum for each protolith was determined using its calculated concentrations of U, K, and Th, and density, using the equation originally proposed by Birch (1954) and modified after (Rybach, 1988):

$$A = \rho \times (0.0952 \times C_U + 0.0348 \times C_K + 0.0256 \times C_{Th})$$

Where A is heat production in $\mu\text{W}/\text{m}^3$, ρ is density in g/cm^3 , and C_U , C_K , and C_{Th} are concentrations of radioactive isotopes of U, K, and Th in ppm, wt. % and ppm, respectively. The calculated results are shown in Figs. 9–10 and Table S4. For a closed-system metapelite, the heat production would depend entirely on the change in density, given the inability for heat-producing radionuclides to leave when dissolved in a melt fraction. As such, this calculated value for A shows a continuous and smooth decrease from 2.32 to 2.17 $\mu\text{W}/\text{m}^3$, although this is unrealistic based on the unrealistic assumption of wholesale melt retention just noted. In contrast, the heat production of a pelite residuum in a conditionally open system shows a step-like decrease from 2.32 to 1.24 $\mu\text{W}/\text{m}^3$. For metabasalt, the heat production shows an almost unchanged value of $A = 0.08 \mu\text{W}/\text{m}^3$ with temperature increase in a closed system, since the concentrations of radioactive isotopes are fixed, but shows a step decrease from 0.08 to 0.03 $\mu\text{W}/\text{m}^3$ in an open system.

5 PATH 2 – CRUSTAL THICKENING FOLLOWED BY SLOW EROSION

5.1 Phase diagrams

Figure 11 and Figure 12 shows mosaic pseudosection panels for the metapelite and metabasalt bulk compositions during crustal thickening followed by slow erosion (P – T path 2). Modebox diagrams are shown below the P – T diagrams.

For the metapelite, the pseudosection panel at the lowest temperature is very similar to that in P – T path 1, except the bulk composition used for modeling contains a slighter lower H_2O content to ensure the solidus is just saturated. During prograde metamorphism, the proposed compression–heating P – T path closely follows contours for mol. % of melt, leading to little melt generation until muscovite dehydrates to form peritectic K-feldspar and melt. The first MLE occurs at 800 °C and 1.27 GPa, and MLE 2 occurs almost immediately afterwards at 802 °C and 1.28 GPa. This supports other studies showing that muscovite dehydration melting can generate voluminous melt over a small temperature range. After muscovite is totally consumed, MLE 3 at 824 °C and 1.38 GPa occurs due to biotite breakdown, which also produces peritectic garnet. No other melt event is calculated to happen before reaching peak P – T conditions. During the decompression stage, the melt generation rate is extremely low, given the prior consumption of hydrous minerals in the residuum. The terminal MLE occurs at 938 °C and 1.06 GPa, leading to 22 mol. % of melt extracted while following this P – T path. Importantly, Spr + Qz would form at 1000 °C at 0.75 GPa in this depleted bulk composition, whereas Opx + Qz is not predicted. The density of the system increases through each pseudosection panel between MLEs during prograde burial, with step increase at each melt loss event; however, bulk-rock density decreases during decompression until it increases sharply at the final MLE. The minimum and maximum density of the system during this evolution are 2.84 g/cm³ at the solidus and 3.06 g/cm³ at peak conditions.

For metabasalt, a total of four pseudosection panels are shown in Figure 12, corresponding to three MLEs. The pseudosection panel at the lowest temperature is the same as that for P – T path 1, except it covers a larger P – T range. MLE 1 occurs at 806 °C and 1.32 GPa, whereas MLE 2 occurs close to peak metamorphism at 847 °C at 1.48 GPa, with the mineralogy of the residuum representing high-pressure granulite. During decompression, the final MLE occurs at 906 °C at 1.22 GPa. Orthopyroxene stabilizes at 930 °C at 1.10 GPa, indicating a transition from high-pressure granulite to intermediate-pressure granulite facies, *sensu stricto*. The P – T path crosses the elevated residuum solidus at 942 °C at 1.04 GPa, which would cause the rock to remelt at 989 °C at 0.81 GPa. The change of density of the residua shows a similar trend to that of the metapelite, with maximum of 3.27 g/cm³ at peak condition and 3.03 g/cm³ at initial solidus conditions.

5.2 Melt and residuum compositions

Changes in the major oxide compositions of the pelitic residua determined via phase diagram modeling show monotonic trends similar to those for P – T path 1, even though the degree of melt loss is subdued (Figure 5). The extracted melts show irregular compositional characteristics as temperature increases: especially the final melt fraction (Figure 6). For metabasalt, the change in major oxide compositions resemble those documented for P – T path 1, except that Al₂O₃ decreases in a step-like fashion due to melt loss, instead of an overall increase (Figure 7). Compared with the extracted melts in P – T path 1, the chemical compositions of extracted melts in P – T path 2 also show irregular evolution as temperature increase.(Figure 8).

For trace element modeling, the concentration of U in the metapelite residuum shows a step-like decrease. By contrast, Th shows a slight increase after MLE 1 and a step-like decrease

thereafter (Figure 9). U and Th concentration in the metabasaltic residua both show stepping decreases as metamorphism progresses (Figure 10).

5.3 Heat production values

Using the heat production equation given above, the pelitic residuum shows an increase from $A = 2.30 \mu\text{W}/\text{m}^3$ to $A = 2.38 \mu\text{W}/\text{m}^3$ during prograde metamorphism before MLE 1. The heat production then decreases to $1.18 \mu\text{W}/\text{m}^3$ during heating up to 1000°C (Figure 9), as heat-producing elements preferentially partition into the melt phase and leave the local environment. For metabasalt, the heat production shows a smooth increase from 0.08 to $0.09 \mu\text{W}/\text{m}^3$ before the first melt extraction, and decreases to $0.04 \mu\text{W}/\text{m}^3$ thereafter (Figure 10).

6 PATH 3 – MULTI-STAGE METAMORPHISM

6.1 Phase diagrams

Figure 13 and Figure 14 show integrated pseudosections for the metapelite and metabasalt. Mineral proportion vs. temperature diagrams during prograde compression-heating and isobaric heating after isothermal decompression are shown below the P – T diagram, and pressure vs. mineral proportion diagrams during isothermal decompression after peak conditions are shown next to the P – T diagram.

Given that the prograde P – T path considered here is the same as the prograde portion of P – T path 2, the melt loss events during this stage are identical in both situations. Thus, we discuss the evolution of both rocks during the latter (decompression) stages of this path. After reaching peak metamorphism, isothermal decompression would induce minor melt generation owing to the negative dP/dT slopes of melt production isopleths associated with phyllosilicate breakdown in the metapelite. The final MLE occurs during the isobaric heating segment at P – T

conditions of 881 °C and 0.75 GPa. The density of the residuum continues to decrease during isothermal decompression, and shows a smooth decrease during isobaric heating in each pseudosection panel. A sudden increase is noted at each MLE, and the maximum and minimum values within this range are the same as those for P – T path 2.

For the metabasalt, the solidus is reached during isothermal decompression at 1.44 GPa and 850 °C owing to its negative dP/dT slope. Orthopyroxene is stabilized and marks the transition to intermediate-pressure granulite at 0.99 GPa and 850 °C, and garnet completely destabilizes at 0.89 GPa and 850 °C. The rock would begin to melt during isobaric heating at 860 °C and 0.75 GPa, and two melt loss events would occur at 941 °C and 995 °C. The density of the system would continuously decrease during ITD, but shows a step-like increase during isobaric heating. The change of density of the residua is the same as those in P – T path 2.

6.2 Melt and residuum compositions

Since the prograde P – T segment in P – T path 3 is the same as that for P – T path 2, geochemical variation within the system for both protolith types would be identical to those discussed previously. After peak metamorphism, the major oxide bulk composition of the pelitic residuum shows a steady change following the first three melt loss events (Figure 5). The final melt extracted along P – T path 3 has a higher SiO_2 , MgO but lower Al_2O_3 , CaO than the final melt extracted along P – T path 2, whereas other elements are similar (Figure 6). The change in major element bulk composition of the basaltic residuum and melt are similar to those in P – T path 1 (Figure 7 and Figure 8). For the trace element contents, U and Th in both pelitic and basaltic residua show step-like decreases after the first melt loss events, but no change afterwards (Figure 9 and Figure 10).

6.3 Heat production values

The heat production capacities of the pelitic and basaltic melt-depleted residua before reaching peak metamorphism are identical to those calculated for P – T path 2. After peak metamorphism, both show a step-like decrease to $1.39 \mu\text{W}/\text{m}^3$ and $0.03 \mu\text{W}/\text{m}^3$, respectively, as a result of extensive melt loss (Figure 9 and Figure 10).

7 DISCUSSION

7.1 Uncertainties associated with forward modeling

Given that investigation of these tectonic models using practical techniques, such as high-temperature experimental petrology, is complicated by the geological necessity of repeated melt loss during burial and exhumation, we approach this problem using theoretical modeling techniques instead. However, it is well known that the modeling approach applied here carries various forms of uncertainty associated with (1) the bulk compositions selected for modeling; (2) the thermodynamic properties of end-members in the petrological data set; (3) the validity of a – x relations that describe mixing between end-members in a single phase; (4) the suitability of solubility models for accessory minerals; and (5) values for trace element partition coefficients. The magnitudes of each are themselves largely unconstrained (Powell & Holland, 2008), although many can be minimized to reduce overall uncertainty related to model results.

The initial compositions selected for phase equilibria modeling are a primary control on the topology of the phase diagram. As a result, the melt compositions generated during partial melting would be different if the protolith composition is different. In addition to major composition, the Zr, LREE, and P_2O_5 would have a significant effect on the amount of accessory minerals in the residue (Kelsey et al., 2008; Yakymchuk et al., 2017). In this study, averaged

pelitic and basaltic bulk compositions were selected for modeling, which thus have implications for typical melt behavior and chemical composition evolution in the crust. Higher Zr and LREE concentrations in the protolith would allow more zircon and monazite to remain in the residue. Consequently, internal heat production might remain high, even at UHT conditions. It would also be reasonable that UHT granulites would have a higher heat production if the protolith had a higher initial U and Th content, although a recent evaluation of the geochemistry of global rocks types shows that the most post-Archean shales have similar values (e.g. Gard *et al.*, 2019).

The most up to date internally consistent dataset available to investigate phase equilibria in metamorphic rocks (ds62: Holland & Powell, 2011) was used in this study, as were the latest *a-x* relations for constraining subsolidus and suprasolidus metamorphism of metapelite and metabasalt (White *et al.*, 2014; Green *et al.*, 2016). While uncertainties (2) and (3) noted above represent the largest sources of error in any single phase diagram (Powell & Holland, 2008), using the same thermodynamic dataset reduces the relative uncertainty between models to around ± 20 °C and ± 0.2 kbar (e.g. Palin, Weller, Waters, & Dyck, 2016; Huang *et al.*, 2018). These values are sufficiently small to be disregarded as having a major influence on the calculated melt production and heat budget of each lithology.

For accessory mineral solubility modeling, we assumed that Zr, LREE, and P only reside in the accessory minerals zircon, monazite and apatite in metapelites, and zircon and apatite in metabasalts. In addition, no accessory minerals or major rock-forming mineral were considered to be carried away as entrained grains with extracted melt. This latter assumption is necessary to estimate the proportion of accessory minerals in the residuum. Here, we use the most commonly adopted zircon solubility model from Boehnke *et al.* (2013), which has been used in many such studies on zircon behavior during partial melting in the past decade (e.g. Yakymchuk & Brown,

2014b; Yakymchuk *et al.*, 2018). For monazite, we selected the solubility equation from Stepanov *et al* (2012) instead of Kelsey, Clark, & Hand (2008), as the former is more sensitive to temperature and the hydration state of the anatectic melt than the latter. Saturation equations for apatite have been defined by Harrison & Watson (1984) and Wolf & London (1994), although the latter was defined at low pressure (2 kbar) for peraluminous melt with $ASI > 1.1$, which would not be suitable for the modeling of metabasalt. In addition, the melt derived from metapelite partial melting at high pressure usually has compositions with $ASI < 1.1$ (Yakymchuk, 2017; Yakymchuk *et al.*, 2018). Therefore, the apatite solubility model from Harrison & Watson (1984) was selected for the modeling in this study.

For modeling of U and Th concentrations, we did not consider potential U and Th host accessory minerals that are stable at subsolidus conditions, such as allanite and xenotime (e.g. Engi, 2017; Finger, Krenn, Schulz, Harlov, & Schiller, 2016; Spear & Pyle, 2010). Allanite is usually found in Ca-rich rocks at amphibolite-facies conditions in the crust, whereas it is not expected to coexist with melt at granulite-facies (or higher) metamorphic grades. As such, U and Th partition coefficients between mineral and melt – and their initial concentrations in the rock – are the major factors that affect the potential thermal capacity of the metamorphic products. The partition coefficients used in this study are constants typical for metapelite and metabasalt, except those between zircon and pelite-derived melt, which are functions of temperature (Kirkland, Smithies, Taylor, Evans, & McDonald, 2015). No partition coefficients for U and Th between muscovite and pelitic melt were assigned due to the lack of experimental data describing these relationships, which may potentially induce some errors, although muscovite is shown to destabilize very soon after partial melting begins. Thus, this is not expected to be an issue for values calculated for UHT conditions.

7.2 Implications for partial melting in the crust

Since fluid-absent dehydration melting plays a primary role in the generation of granite (e.g. Brown, 2013; Clemens, 2012; Sawyer *et al.*, 2011), rocks containing large volumes of hydrated minerals, such as muscovite, biotite, and hornblende, play significant roles in crustal differentiation during anatexis (Yakymchuk, 2019). Based on this assumption, amphibolite-facies metapelites, rich in mica, and metabasalts, rich in hornblende, were used to model the petrological evolution of a crustal column during metamorphism along various P – T paths.

Partial melting of a metapelite during isobaric heating at 0.8 GPa produces up to 70 vol. % of melt at 1000 °C in a closed system environment, but only 27 vol. % of cumulative melt in open system environment that allows sequential pulses of melt to leave the system once a critical threshold is reached. These results resemble anatexis in metabasalt, which generates 35 vol. % of melt up to 1000 °C during isobaric heating in a closed system, but only 22 vol. % of melt in an open system. Both results confirm the interpretations of previous models that progressive melt extraction significantly decreases the fertility of the remaining migmatite (Yakymchuk & Brown, 2014a). In fact, melt extraction at an MCT of 7 vol. % is suggested to occur in the absence of syn-anatectic deformation (Rosenberg & Handy, 2005; Vigneresse, Barbey, & Cuney, 1996), and this threshold would likely to be lower in deforming rocks (Brown, 2010). Once a permeable network of partial melt is developed, the positive volume change of the system due to melt generation and viscosity difference between melt and solid residuum would promote melt exfiltration from the system and ascent to shallower crust driven by buoyancy (Clemens & Droop, 1998; Rutter & Mecklenburgh, 2006). Thus, modeling of partial melting in conditional open systems is most realistic for simulating natural tectonic processes.

Modeled P – T path 1 corresponds to thermal metamorphism associated with mantle upwelling (Sizova *et al.*, 2014). In this scenario, all melt lost from the metapelite protolith is granitic and alkaline in composition, with systematic changes of elements as a function of temperature (Figure 15). All the melt compositions are peraluminous with ASI >1.1. As a result, a total of 27 vol. % of S-type granite would be generated. The compositions of extracted melts from metabasalt are all subalkaline and metaluminous, evolving from I-type granite to monzonite as temperature increases. Thus, 17 vol. % of I-type granite and 5 vol. % of monzonite would be produced at this tectonic setting.

In a tectonic setting involving crustal thickening followed by slow erosion (Clark *et al.*, 2011), the metapelite-derived melts also have granitic and alkaline partial melts, but the ASI of the first two pulses are below 1.1. This produces 22 vol. % of S-type granite during partial melting of metapelite along this P – T path. For metabasalt, three extracted melt fractions constitute 17 vol. % of the initial protolith and are all subalkaline granites with ASI values ~ 1.0.

For modeling of a multi-period thermal anomaly (Huang *et al.*, 2019), melts extracted during prograde metamorphism are the same as those documented for P – T path 2. During subsequent isobaric heating at 0.75 GPa, the final extracted melt fraction from the metapelite is alkaline, granitic and peraluminous. In contrast, the final two extracted melt fractions from the metabasalt evolve from monzonitic to monzodioritic composition, with both being subalkaline and metaluminous. As a result, 22 vol. % of S-type granite would be formed from partial melting of metapelite, and 12 vol. % of I-type granite, 5 vol. % of monzonite, 5 vol. % of monzodiorite would be produced from partial melting of metabasalt in this tectonic setting.

As the densities of extracted melts are always lower than those of the residua, melt generated at this middle to lower crustal setting will ascend to shallower levels, driven by

buoyancy (Brown, 2013; Yakymchuk, 2019; Yakymchuk & Brown, 2014a). The emplacement and eruption of these granitic, dioritic, and gabbroic magma then drives inter-crustal differentiation, changing the composition of the upper continental crust through time and generally causing it to become more silica-rich (felsic), whereas silica-poor residua are left behind and drive the middle to lower crust to more basic compositions (Sawyer et al., 2011). Basalt-derived melts generated at high pressure and all pelite-derived melts are granitic, but basalt-derived melts generated from middle crust are much more mafic, especially at high temperature. It might be plausible that the volume fraction of mafic rocks in the middle crust would be important for determining the maficity of the upper crust. However, the modeling in this study only considers melt internally derived from granulite. In reality, magma mixing among melts derived from various sources is ubiquitous in granulite and UHT terranes. In a crustal thinning and mantle underplating scenario, some granite is usually generated by mixing of metamorphic melts and juvenile mafic magma, as well as significant amount of residua (Korhenon et al., 2015; Wang et al., 2018). Thus, we can only suggest the volume fraction of mafic rocks in the middle crust that might contribute to the maficity to the upper crust, but in reality magmatism would be much more complicated than our modeling. These data may therefore be considered as an ideal end-member scenario upon which more complex modeling studies may be built.

7.3 Implications for identifying UHT metamorphism in the rock record

As UHT granulites usually experienced extensive partial melting and melt loss, it is difficult to constrain the exact P – T path, melt composition or melt volume that was lost during the prograde stage. In this study, we proposed several possible P – T paths that UHT granulite might experience and used unconventional panel diagrams to investigate the melt behavior and

chemical composition evolution along these P – T paths, which have some theoretical implications for the study of UHT metamorphism. Nonetheless, these assumed processes might be more complicated in natural systems.

Here, for a conventional (closed-system) phase diagram analysis, the diagnostic UHT mineral pairing Spr + Qz is not predicted to form in metapelitic rocks at high grade conditions (Figure 1), but high-Al orthopyroxene + sillimanite stabilizes in a restricted P – T range of 1000–1020 °C, 0.69–0.72 GPa. This indicates that a protolith must already be Mg-rich to be able to generate this diagnostic UHT mineral assemblage, even though the P – T range is narrow. In contrast, Spr + Qz does occur over a wide P – T range under open-system conditions along several P – T paths (Figures 3, 11, and 13). However, other UHT diagnostic mineral assemblages, such as high-Al orthopyroxene + sillimanite, are not predicted to form under open-system conditions, which is a constraint of the effective bulk composition. We find a progressively increasing concentration of Al₂O₃ and MgO in their respective residues: an effect that is more pronounced at low pressure, owing to more MLEs (Figure 5). The increase of Al₂O₃ and MgO in the residue is due to relatively lower Al₂O₃ and MgO in the melt than the original protolith, as shown by mass balance (Rapp, Ryerson, & Miller, 1987). Thus, whether or not a metapelite can form diagnostic UHT mineral assemblages is primarily controlled by protolith composition, and the degree of melt loss event being a subsidiary effect. In a relatively Mg-rich protolith, open-system metamorphism and melt loss is necessary to form Mg–Al rich domains from metasedimentary protoliths, as hypothesized previously (e.g. Baba, 2003; Brandt *et al.*, 2007; Clifford *et al.*, 1981; Droop & Bucher-Nurminen, 1984; Lal *et al.*, 1978; Raith *et al.*, 1997). If 7 vol. % melt is used as a threshold for accumulation before extraction in quartzofeldspathic lithologies, at least three discrete melt loss events at high pressure (i.e. lower-crustal depth) or discrete four melt loss

events at lower pressure (i.e. middle-crustal depths) are necessary to create these diagnostic UHT assemblages. However, in actively deforming systems, where melt may exfiltrate at lower melt fractions, the same change in residuum composition may be achieved by a more continuous drainage as opposed to discrete pulses.

By contrast with metapelites, open-system vs. closed-system metamorphism and melt loss in metabasaltic compositions are more similar to one another, except for small variations in minor phase concentrations, such as ilmenite and rutile. At least two melt loss events occur prior to reaching UHT conditions along all considered P – T paths. Even though some Mg-rich phases, such as orthopyroxene, are stable at UHT conditions, the overall stability of these minerals extends over a larger P – T range both in closed-system and open-systems, leading to difficulty in identifying UHT conditions in mafic granulites. Compared with the evolution of Al_2O_3 in a pelitic residue, the Al_2O_3 in mafic residua shows a limited change along various P – T paths. The evolution of other elements in the residua usually change consistently up-temperature. Although feldspar may begin to take on characteristics of ternary compositions, this may be lost upon cooling due to retrograde cation equilibration. Thus, in line with the results of previous studies, we find that UHT metamorphism is very difficult to identify in meta-basic rocks, regardless of the degree of melt loss, as the mineral assemblages that occur at lower-granulite facies conditions largely resemble those that stabilize above 900 °C. This result is problematic given the abundance of evidence showing that the lower crust is largely mafic in composition, equivalent to a basaltic andesite. Although the upper and middle crust is more felsic (granitic/pelitic), UHT conditions are significantly more difficult to achieve at these depths, except for unusual circumstances that may lead to temperatures locally exceeding 900 °C around hot and dry magmatic intrusions.

581 This modeling also provides new insight into the thermal energy budget of partially
582 melted rocks in the lower crust. Some researchers have proposed a high content of heat
583 producing elements at such depths, which could generate $>3.5 \mu\text{W}/\text{m}^3$ and so possibly induce
584 UHT conditions in regions with low erosion rates ($<0.05 \text{ mm}/\text{y}$) (e.g. Clark *et al.*, 2011).
585 However, the heat production values calculated in this study show an overall decrease with
586 temperature in various tectonic settings, even though volume reduction during burial due to melt
587 loss acts to slightly increase heat production owing to an increase in density (Figure 9 and Figure
588 10). These calculated results show similar trends in metapelitic and metabasaltic lithologies,
589 although heat production values for the latter are extremely low ($<1.0 \mu\text{W}/\text{m}^3$) regardless, such
590 that they would make no realistic contribution to increasing or sustaining high temperatures in
591 the crust.

592 Our modeling results are consistent with the conventional view that there is a downward
593 decrease in the concentration of HPEs in the lower crust, based on seismological evidence and
594 bulk rock composition analyses (Rudnick and Gao, 2014 and references therein). In these works,
595 some lower crust of many Archean cratons (e.g. Kaapvaal craton, North China craton) are
596 characterized by slow *P*-wave velocities and low heat flow, which were interpreted as highly
597 evolved pelitic rocks depleted in HPEs (Durrheim and Green, 1992; Liu *et al.*, 2001; Nguuri *et al.*,
598 2001; Niu & James, 2002). In recent works, however, some chemical analyses and theoretical
599 modeling work suggest a conservation of deep crustal heat production (e.g. Alessio *et al.*, 2018;
600 Yakymchuk & Brown, 2019). Yakymchuk and Brown (2019) interpreted the contradictory
601 between equilibrium modeling and natural rocks reported by Alessio *et al.* (2018) as a result of
602 new monazite growth near the metamorphic peak driven by upward percolation of
603 LREE-saturated melt. Alternatively, phase equilibrium modeling cannot consider the shielding of

accessory mineral grains within porphyroblasts, which removes them from the matrix. As a result, this imbalance at UHT conditions may be resolved. In addition, theoretical modeling also indicates that an initial high LREE concentrations in the protolith would preserve monazite from being totally resorbed at UHT conditions (Kelsey et al., 2008). All of these factors might plausibly explain the slight increase of Th in the residue during heating, but U does decrease up-temperature, as shown from both natural rocks and theoretical modeling (Alessio et al., 2018; Yakymchuk and Brown, 2019). Nonetheless, the heat production rate of Th ($0.072 \mu\text{W m}^{-3}$) is much lower than that of U ($0.265 \mu\text{W m}^{-3}$) (Bea, 2012), therefore bulk-rock heat production would decrease due to U loss, even if Th becomes more concentrated in the residue. Such an occurrence is shown for the metapelitic residue in this work at $< 850^\circ\text{C}$ at 0.8 GPa.

In general, granulite and UHT terranes do not only comprise pelitic and mafic granulites. Granitic rocks, which usually have high heat production, are also often emplaced into these high grade terranes due to earlier metamorphic episodes (Huang et al., 2019). In such cases, all lithologies should be considered when evaluating the contributions of heat production on bulk-terrane heat flow. Based on the review work of granite heat production by Artemieva et al. (2017), granite formed before the Early Proterozoic usually has a low heat production ($< 2 \mu\text{W m}^{-3}$ on average), which increases forwards in time to peak during the Mesoproterozoic ($c. 4.5 \mu\text{W m}^{-3}$ on average). Granite formed after this period of time generally shows a steady decrease in heat production to the present day ($2.7 \mu\text{W m}^{-3}$ in average). Given the pervasiveness of UHT metamorphism in the Precambrian (Brown & Johnson, 2018), we suggest that heat production would not be the only mechanism driving UHT metamorphism on the early Earth, but it must have been a contributor in many cases.

7.4 Implications for heat budget of melting reaction under open-system

Among various lithologies in a granulite-UHT terrane, and assuming the presence of fluid, metapelite is the most fertile rock, metabasites are the second-most fertile, and most other lithologies such as meta-granitoids and meta-sandstone are usually highly refractory. It is well known that a number of subsolidus and suprasolidus metamorphic reactions and melting reactions are endothermic, buffering temperature increase during the heating process (e.g. Bea, 2012; Lyubetskaya & Ague, 2009; Stüwe, 1995; Thompson & Connolly, 1995; Vielzeuf, Clemens, Pin, & Moinet, 1990). As a result, a disparity of peak metamorphic temperature would be revealed among various lithologies, among which metapelite usually registered the lowest temperature, whereas other refractory rocks record a 60–70 °C higher peak metamorphic temperature (e.g. Namaqua-Natal Metamorphic Complex, South Africa, Schorn & Diener, 2019).

A comparison of enthalpy changes for an average metapelite during prograde metamorphism between closed- and open-system was modeled by Schorn et al. (2018). For open-system conditions, they modeled episodic melt extraction (extracting 5 mol.% melt as soon as threshold of 7 mol.% is reached) and continuous melt extraction (extracting all melt in excess of 2 mol.% threshold as soon as it is produced). Both show consistent enthalpy change with that in a closed-system for major melting reactions (e.g. sillimanite + biotite + quartz \rightarrow garnet + cordierite + K-feldspar + melt). After biotite is totally consumed, the residue in an open system is able to transform heat to temperature more efficiently.

In this study, the temperature at which biotite is totally consumed in an open-system (c. 850 °C at 0.8 GPa) is identical to that in a closed-system, which is consistent with the results by Schorn et al. (2018). From the view of heat transformation to temperature, whether or not melts can drain away from the system will not have a significant influence. However, melt extraction

would strengthen the crust, leading to an increase of mechanical heat production (Clark et al., 2011; Nabelek, Whittington, & Hofmeister, 2010). Given that the production and redistribution of heat in the lithosphere would be a combination of heat conduction, heat advection, and heat production (Stüwe, 2007), we proposed that most UHT metamorphism would be driven by a hybrid mechanism, including advective heat from mantle, radioactive heat production as well as mechanical heat production.

8 CONCLUSIONS

Phase equilibria modeling of open-system melting of metapelite and metabasalt suggest that progressive melt loss events caused by crossing the melt connectivity threshold make a key contribution to intracrustal differentiation, leading to an increase of Al and Mg in metapelitic paleosomes, which provide a possible mechanism for forming sapphirine + quartz in residual Mg–Al rich domains in an originally Mg-rich metasedimentary rocks. Metabasalt assemblages are less sensitive to bulk compositional changes at UHT conditions. More than three and two melt loss events are modeled to occur as the rocks evolve to UHT conditions in pelitic and basaltic bulk compositions, respectively. Partial melting in an open system environment would produce 22–27 vol. % S-type granite and 12–17 vol. % I-type granite, respectively. Further, the heat production values of the residuum would attenuate in an open-system environment. Most UHT metamorphism is likely therefore driven by a combination of advective heat supplied from the mantle, internal radioactive heat production, as well as mechanical heat production.

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SUPPORTING INFORMATION

Additional Supporting Information may be found online in the supporting information tab for this article.

Table S1 Bulk composition used for phase equilibria modeling

Table S2 Modeled results of major composition of extracted melt

Table S3 Modeled amount of accessory minerals in the rocks

Table S4 Modeled U and Th concentrations in the rocks and calculated results of heat production value

FIGURE CAPTIONS

Figure 1 P – T pseudosection calculated for an average amphibolite-facies pelite at closed system, contoured with isopleth of mol. % melt. The black bold solid arrow representing isobaric heating at 0.8 GPa is proposed P – T path 1. The mineral proportion against temperature for isobaric heating at 0.8 GPa is shown below.

Figure 2 P – T pseudosection calculated for an average MORB at closed system, contoured with isopleth of mol. % melt. The bold solid line representing isobaric heating at 0.8 GPa is proposed P – T path 1. The mineral proportion against temperature for isobaric heating at 0.8 GPa is shown below.

Figure 3 P – T mosaic pseudosection panels of metapelite at open system along proposed P – T path 1, contoured with isopleth of mol. % melt. The mineral proportion against temperature is shown below.

Figure 4 P – T mosaic pseudosection panels of metabasalt at open system along proposed P – T path 1, contoured with isopleth of mol. % melt. The mineral proportion against temperature is shown below.

Figure 5 The evolution of the compositions of the metapelite along various P – T paths against temperature.

Figure 6 The evolution of composition of extracted melts from metapelite along various P – T paths against temperature.

Figure 7 The evolution of the compositions of the metabasalt along various P – T paths against temperature.

Figure 8 The evolution of composition of extracted melts from metabasalt along various P – T paths against temperature.

Figure 9 Modeled U, Th, K concentrations in the pelitic residual and calculated results of heat production values.

Figure 10 Modeled U, Th, K concentrations in the basaltic residual and calculated results of heat production values.

Figure 11 P – T mosaic pseudosection panels of metapelite at open system along proposed P – T path 2, contoured with isopleth of mol. % melt. The mineral proportion against temperature is shown below.

Figure 12 P – T mosaic pseudosection panels of metabasalt at open system along proposed P – T path 2, contoured with isopleth of mol. % melt. The mineral proportion against temperature is shown below.

Figure 13 P – T mosaic pseudosection panels of metapelite at open system along proposed P – T path 3, contoured with isopleth of mol. % melt. The mineral proportion against temperature is shown below.

Figure 14 P – T mosaic pseudosection panels of metabasalt at open system along proposed P – T path 3, contoured with isopleth of mol. % melt. The mineral proportion against temperature is shown below.

Figure 15 Geochemical classification diagrams for extracted melts. (a) Total alkali against silica diagram (TAS, after Middlemost, 1994) for metapelite-derived melts; (b) A/NK against A/CNK classification diagram (Maniar & Piccoli, 1989) for metapelite-derived melts; (c) TAS diagram for metabasite-extracted melts; (d) A/NK against A/CNK classification diagram for metabasite-extracted melts. Compositions of melts generated along $P-T$ path 1 to $P-T$ path 3 for open system are labeled with orange cubes, grey triangles and yellow circles, respectively.