Timing of partial melting and granulitisation during the formation of high to ultra-high temperature terranes: insight from numerical experiments – Cenki, Rey, Arcay and Giordani.

SUPPLEMENTAL FILES

TABLE DR1. THERMAL AND MECHANICAL PARAMETERS

Parameter	Continental Crust (CC)	Sediments	Retrogressed CC	Granulitic CC	Upper Mantle
Reference temperature (K)	293	293	293	293	293
Dislocation creep viscous rheology	Wet quartzite[a]	Wet quartzite[b]	Wet quartzite[a]	Dry Maryland Diabase[c]	Isoviscous (5.10^{21} Pa.s)
Reference density ($kg \cdot m^{-3}$)	2600	2300	2600	2950	3370
Thermal expansivity (K-1)	-	-	-	-	2.80E-05
Beta (Pa^{-1})	-	-	-	-	-
Heat capacity ($J\ K^{-1}\ kg^{-1}$)	1000	1000	1000	1000	1000
Thermal diffusivity ($m^2\ s^{-1}$)	1E-06	1E-06	1E-06	1E-06	1E-06
Latent heat of fusion ($kJ\ kg^{-1}\ K^{-1}$)	250	250	250	250	-
Total radiogenic heat production ($W\ m^{-3}$)[d]	1.0483E-06/2.0922E-06	0.7E-06	1.0483E-06	1.0483E-06	-
Melt fraction density change[e]	0.13	-	0.13	0.13	-
Solidus term 1 (K)	923	-	923	1263	-
Solidus term 2 ($K\ Pa^{-1}$)	-1.20E-07		-1.20E-07	-1.20E-07	-
Solidus term 3 ($K\ Pa^{-2}$)	1.20E-16	-	1.20E-16	1.20E-16	-
Liquidus term 1 (K)	1423	-	1423	1763	-
Liquidus term 2 ($K\ Pa^{-1}$)	-1.20E-07	-	-1.20E-07	-1.20E-07	-
Liquidus term 3 ($K\ Pa^{-2}$)	1.60E-16	-	1.60E-16	1.60E-16	-
Friction coefficient	0.44	0.12	0.44	0.44	0.44
Softened friction coefficient	0.088	0.02	0.088	0.088	0.088
Cohesion (MPa)	15	20	15	15	15
Softened cohesion (MPa)	3	20	3	3	3
Pre-exponential factor ($MPa^{-n}\ s^{-1}$)	6.60E-08	1.1E-22	6.60E-08	5.05E-22	-
Stress exponent (n)	3.1	4.0	3.1	4.7	-
Activation energy ($kJ\ mol^{-1}$)	135	223	135	485	-
Factor	1	1	1	1	-
Activation volume ($m^3\ mol^{-1}$)	0	3.1E-06	0	0	-
Water fugacity	0	0	0	0	-
Water fugacity exponent[f]	0	0	0	0	-
Melt viscous softening factor	1.00E-03	-	1.00E-03	1.00E-03	-
Softening melt fraction interval	0.2-0.3	-	0.2-0.3	0.2-0.3	-

Additional parameters:
Model Size: 480 km length (240 nodes, constant spacing) - 160 km thick (80 nodes, constant spacing) i.e. 20 km air-like material, 33-40 km crust, 100-107 km upper mantle. The marker density is uniform (60 per grid cell).
A zone of damage insures initial heterogeneities in plastic strain in the entire model.
The initial basal heat flow is set at 0.020 $W.m^{-2}$
Isostasy (Mondy et al., 2018) is activated
A model stress limiter is set at 150 MPa (100 MPa for sediments and upper mantle)
Erosion and sedimentation are active with threshold of 4 km and 0 km, respectively
Prograde continental crust to granulite phase change set at 1050 K
Retrograde granulite to retrogressed continental crust phase change set at 1050 K and 10^{-14} s^{-1} strain rate
Moho temperature at the start of the model is *ca*. 650 °C
Solidus and liquidus are defined by a polynomial function of pressure (P):
$T_s = a_0 + a_1 \times P + a_2 \times P^2$, $T_l = b_0 + b_1 \times P + b_2 \times P^2$
The density of the continental crust changes according to T and P:
$\rho = \rho_0 * (1 + (\beta * \Delta P) - (\alpha * \Delta T))$
Note that the presence of melt has an impact on density.
The maximum melt fraction is 30%.

References:
a Parameters were derived from Paterson and Luan (1990)
b Parameters were derived from Gleason and Tullis (1995)
c Parameters were derived from Mackwell et al (1998)
d Parameters were derived from Gard et al (2019). See text for explanation.
e Melt and other parameters were derived from Rey and Muller (2010)
f A zero value denotes that this effect on the viscous flow law is incorporated into the pre-exponential factor

Details of modeling procedures, rheological and thermal parameters:

The layer of air-like material, with low-viscosity and low-density, accommodates the development of surface topography. Surface conditions are defined by the 0 °C isotherm and a free slip surface. Erosion (for material reaching above 4 km) and sedimentation (when the surface of the crust subsides below 0 km) are allowed to take place throughout the model and are modelled as phase changes. Shortening and extensional velocity boundary conditions are imposed on both vertical walls of the model. Horizontal boundaries of the model are free slips. The conditions at the base of the model are controlled by isostasy (Mondy *et al.*, 2018). The thermal properties of the materials (total *RHP*, *RHP* distribution) vary between the experiments but the initial *BHF* is kept constant (0.020 $W.m^{-2}$) and the initial steady-state geotherm always delivers a temperature at the Moho close to ~ 650 °C. We select from the literature realistic visco-plastic parameters so that the mechanical behavior of the modeled crust depends on temperature, strain rate, deviatoric stress and accumulated strain, and phase transitions. As this study focusses on the crust, mantle viscosity has been simplified and is considered isoviscous ($5*10^{21}$ Pa.s after having tested several values yielding similar results). In order to explore the interplay between partial melting and the formation of granulites, we have parameterized first-order metamorphic phase transitions as in Cenki-Tok *et al.* (2020).

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