Supporting Information for

Subduction evolution controlled Himalayan orogenesis: Implications from 3-D subduction modeling

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1. Methods and model setting

Based on the thermomechanical model Stag3d [11] and the finite difference method (FDM), we investigate the in situ along-strike slab thermal variation in megathrusts and the petrological metamorphic changes in the incoming oceanic lithosphere. An anelastic liquid approximation and the equations of conservation of mass, momentum, and energy are used in this study:

$$\nabla \cdot \{\rho_s(z, T_s)\boldsymbol{v}\} = 0, \tag{S1}$$

$$-\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} - \delta_{i3}\rho_s g\alpha_0(T - T_s) = 0, \tag{S2}$$

$$\rho c_p(\frac{\partial T}{\partial t} + \boldsymbol{v} \cdot \nabla T) = k\nabla^2 T + \eta(\nabla v)^2 + \rho g\alpha T v_z + \rho H_r, \tag{S3}$$

where P is the pressure deviation from hydrostatic pressure, α_0 is the reference thermal expansivity, τ_{ij} (i,j = 1, 2, 3) is the stress tensor, and δ_{ij} is the Kronecker delta. The energy equation includes the advection term, thermal diffusion term, viscous dissipation term, adiabatic heating term, and radioactive heating term. The main model parameters are tabulated in Tables S1–S2 (SI).

The viscous flow law for wet olivine [42] following laboratory experiments is included in this study. The deformation of olivine occurs by both diffusion creep (df) and dislocation creep (ds), where each mechanism accommodates a portion of the total strain rate [43]:

$$\dot{\varepsilon}_t = \dot{\varepsilon}_{df} + \dot{\varepsilon}_{ds}. \tag{S4}$$

The composite upper mantle viscosity under a given condition is

$$\eta_{comp} = \frac{\eta_{df}\eta_{ds}}{\eta_{df}+\eta_{ds}}, \tag{S5}$$

where η_{df} and η_{ds} are the diffusion creep and dislocation creep viscosities for olivine, respectively. The general viscosity law is

$$\eta_{df,ds} = \left(\frac{d^p}{A_0 C_{OH}^r}\right)^{\frac{1}{n}} \dot{\varepsilon}_E^{\frac{1-n}{n}} exp\left(\frac{E_0+P_l V_0}{n_0 R T_a}\right). \tag{S6}$$

Here, $\dot{\varepsilon}_E = (\frac{1}{2}\dot{\varepsilon}_{ij}\dot{\varepsilon}_{ij})^{\frac{1}{2}}$ is the square root of the second invariant of the strain rate tensor (e.g., [44]), T_a is the absolute temperature, R is the gas constant, and P_l is the lithostatic pressure. The values of the model parameters for the diffusion and

dislocation creep of olivine are tabulated in Table S1. The trenchward thermal structure follows the Global Depth and Heat (GDH1) model [16,45]:

$$T(z,t_{oc}) = T_m\left[\frac{z}{d_0} + \frac{2}{\pi}\sum_{n-1}^{\infty}\frac{1}{n}\sin(\frac{n\pi z}{d_0})\exp(\frac{-n^2\pi^2\kappa t_{oc}}{{d_0}^2})\right] \quad \text{(S7)}$$

The time-dependent thermal boundary condition includes the initialization time. $T(z,t_{oc})$ is the temperature at depth z and plate age t_{oc} along the trench, T_m is the lithospheric basal temperature, κ is the thermal diffusivity, and d_0 is the adiabatic heating layer minimum depth.

The model involves 3-D geometric data for the incoming plate updated through seismic tomography (Slab2, [14]) and real subduction velocities prescribed or based on the MORVEL [17,18] data sets. The slab topography with a depth of 60~100 km are extrapolated and is assumed to feature steep subduction (45^o) before 42 Ma (Fig. 2) and shallow subduction (15^o) after 42 Ma. The age of the oceanic plate follows the oceanic seafloor age according to EarthByte [46] estimated at the trenchward model boundary. The thickness of the incoming plate is estimated according to the plate age [15]. The incoming oceanic plate is composed of a MORB layer at the top with a thickness of 7 km underlain by an ultramafic rock layer [47]. The temperature boundary condition agrees with the plate cooling model [16]. The bottom of the slab and the perpendicular plane are prescribed as adiabatic and permeable, and the top surface is set to be a fixed temperature (0°C) and permeable. The subduction velocities inside a prescribed 3-D constrained volume of the oceanic lithosphere are given based on the kinematic plate subduction modeling method [12,48]:

$$v_x(x,y,z) = \frac{-2a(x,y)b(x,y)v_y + \sqrt{\{2a(x,y)b(x,y)v_y\}^2 - 4\{a(x,y)^2+1\}[\{a(x,y)^2+1\}v_y{}^2 - v^2]}}{2\{a(x,y)^2+1\}}, \quad \text{(S8)}$$

$$v_y(x,y,z) = v_y, \quad \text{(S9)}$$

$$v_z(x,y,z) = a(x,y)v_x + b(x,y)v_y, \quad \text{(S10)}$$

while

$$a(x,y) = \frac{1}{2}\{Z(x+\Delta x,y) - Z(x-\Delta x,y)\}\cdot\frac{z_{max}}{x_{max}}, \quad \text{(S11)}$$

$$b(x,y) = \frac{1}{2}\{Z(x+\Delta x, y+\Delta y) - Z(x+\Delta x, y) + Z(x-\Delta x, y) - Z(x-\Delta x, y-\Delta y)\} \cdot \frac{z_{max}}{y_{max}}. \quad \text{(S12)}$$

Here, v is the subduction velocity, and Δ is the interval between two neighboring nodes along the axes. x_{max}, y_{max}, and z_{max} indicate the model lengths along the x, y, and z axes, respectively.

Observations of surface heat flow from the Global Heat Flow Database [49] and heat flow values from Curie point depth estimates [50] are used to constrain the model. Our model follows the trench temperature boundary of the plate cooling model [16,45]. We prescribe the subduction time to be at least 20 Myr to ensure that the model reaches a steady thermal state with a temperature variation < 10°C over time with a lapse time of ≥ 5 Myr. We tested the resolution and found that the temperature variance was < 1% with a maximum temperature variance < 1.9% between meshes of 80 × 80 × 100 and 96 × 96 × 100. We performed sensitivity tests to investigate the robustness of our modeling results and varied the mantle viscosity from 1.0×10^{19} Pa s to 1.0×10^{21} Pa s and the mantle density from 3250 kg/m^3 to 3350 kg/m^3. We present the benchmark model results as deviations from the reference models (ΔT and ΔH_2O) and show these results at different depth levels within the oceanic slab. The tests show that mantle density variations (±50 kg/m3) induce small temperature variations of <10°C at depth.

Surface heat flow and Curie depth are correlated, following a theoretical thermal conduction relationship (e.g., [51]):

$$Q_s = K\frac{T_c - T_0}{Z_b - Z_s} + h_r^2 H_0 \frac{e^{\frac{-Z_b}{h_r}} - e^{\frac{-Z_s}{h_r}}}{Z_b - Z_s} + h_r H_0 e^{\frac{-Z_s}{h_r}} \quad \text{(S13)}$$

where Q_s is the surface heat flow, T_c is the Curie temperature at the Curie depth Z_b, T_0 is the temperature at the surface elevation Z_s, K is the average thermal conductivity of the magnetic layer, H_0 is the heat production rate at the surface, and h_r is the characteristic drop-off of heat production. The equation shows a nonlinear inverse

relationship between heat flow and Z_b. For the oceanic lithosphere, we assume $H_0 = 1.37\ \mu W/m^3$, $h_r = 5.0$ km, $T_c = 550$ °C, $T_0 = 5$ °C, and $Z_s = 4$ km. For continents, we take $H_0 = 2.0\ \mu W/m^3$, $h_r = 10.0$ km, and $Z_s = -1$ km to account for the larger radioactive contribution [52]. High heat flow measurements tend to correlate with small Curie depths, and vice versa. The continental data can be best fitted with the theoretical curve of an average thermal conductivity K of ~2.5 W/m°C, and most oceanic data are best fitted with an average K = ~2.0 W/m°C [51]. These conductivities are compatible with those of granite and basalt (e.g., [52]). The synthetic modeling suggests that the largest error in the estimated Curie depths using the linearized centroid method will not reach 35%, and the uncertainty of the surface heat flow is expected to be <20 mW/m^2 due to the selected fractal exponent and wavenumber bands for linear regressions and observed surface heat flow in plate convergence zones (e.g., [50,51]).

The erosion rate is prescribed according to the monsoon intensity and height dependent parameters (Table S1) for each grid on the model surface at each timestep. Then, the height of the grids on the surface at this timestep is reduced by the effect of erosion in a vertical distance (that is calculated via multiplying the prescribed erosion rate and the length of interval time before this timestep) to obtain the grid net height. Then the net height of surface grids are put into the next iterative calculation until the next timestep. Through such iteration, we are enabled to estimate the effect of erosion rate on surface topography of the overriding plate.

The other model settings combine effective simulation methods used in active convergence zones, such as the reconstruction of oceanic-continental cold subduction in eastern Japan [48,53], Hikurangi [54], and Sumatra [10] and warm subduction in southwestern Japan [12,55], Ryukyu [56], and Cascadia [57]. These studies on 3-D thermomechanical models are focused on subducted plates with topographically changing dip angles.

Table S1 Main model parameters

	Model Parameters	Value	Units
ρ_0	Standard density	3300 [58]	$kg{\cdot}m^{-3}$
α_0	Standard thermal expansion	3×10^{-5} [59]	K^{-1}
T_0	Standard temperature	1600	K
k_0	Standard thermal conductivity	2.9 [60]	$W{\cdot}m^{-1}{\cdot}K^{-1}$
Hr	Radioactive heat generation rate in the mantle	2.245×10^{-13} [58]	$W{\cdot}m^{-3}$
C_{p_0}	Standard specific heat at constant pressure	1200 [58]	$J{\cdot}kg^{-1}{\cdot}K^{-1}$
κ_0	Standard thermal diffusivity	7.6×10^{-7} [13]	$m^2{\cdot}s^{-1}$
η_0	Standard viscosity	1×10^{20} [60]	Pa·s
v	Subduction velocity:	4.4~11.8 [18]	$cm{\cdot}y^{-1}$
	60 Ma~42 Ma	11.8	$cm{\cdot}y^{-1}$
	42 Ma~23 Ma	8.3	$cm{\cdot}y^{-1}$
	23 Ma~11 Ma	5.7	$cm{\cdot}y^{-1}$
	11 Ma~0 Ma	4.4	$cm{\cdot}y^{-1}$
v	Surface erosion rate:	(0.2~0.4)*h [19]	$mm{\cdot}y^{-1}$
	60 Ma~42 Ma	0.2	$mm{\cdot}y^{-1}$
	42 Ma~23 Ma	0.3	$mm{\cdot}y^{-1}$
	23 Ma~11 Ma	0.4	$mm{\cdot}y^{-1}$
	11 Ma~0 Ma	0.3	$mm{\cdot}y^{-1}$
		Diffusion Creep [43]	Dislocation creep [43]
n_0	Stress exponent	1.0	3.5
A_0	Preexponential factor	1.0	9.0×10^{-20}
C_{OH}	OH concentration (H/10^6 Si)	1000	1000
r	C_{OH} exponent	1.0	1.2
E_0	Activation energy (kJ/mol)	335	480
V_0	Activation volume (m^3/mol)		
	Upper mantle	4.0×10^{-6}	11.0×10^{-6}
	Lower mantle	1.5×10^{-6}	-
d	Grain size (μm)		
	Upper mantle	10,000	-
	Lower mantle	40,000	-

h=[height(m)/10^3]×(2.7/0.6)×(T_{uplift}/T_{all}) [19]

Table S2 Parameters for model domains

Domains	Upper crust	Lower crust	Slab	Mantle
Thickness (km)	20	20	50	>300
Density (kg/m^3)	2600	2900	3300-3800	3300
Viscosity (Pa·s)	∞	1.0×10^{19}	1×10^{20}	1×10^{20}
Elastic modulus (GPa)	98	98	100	170