Stress and strain during fault-controlled lithospheric extension—insights from numerical experiments

Andreas Henk*

Geologisches Institut, Universität Freiburg, Albertstr. 23 b, D-79104 Freiburg, Germany

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Abstract

Two-dimensional finite element techniques are used to study the temporal evolution and spatial distribution of stress and strain during lithospheric extension. The thermomechanical model includes a pre-existing fault in the upper crust to account for the reactivation of older tectonic elements. The fault is described using contact elements which allow for independent meshing of hanging wall and foot wall as well as simulation of large differential displacements between the fault blocks. Numerical models are run for three different initial temperature distributions representing extension of weak, moderately strong and strong lithosphere and three different extension velocities. In spite of the simple geodynamic boundary conditions selected, i.e., wholesale extension at a constant rate, stress and strain vary substantially throughout the lithosphere. In particular, in case of the weak lithosphere model, lower crustal flow towards the locus of maximum upper crustal extension results in the formation of a lower crustal dome while maintaining a subhorizontal Moho relief. The core of the dome experiences hardly any internal deformation, although it is the part of the lower crust which is exhumed the most. Stress fields in the lower crustal dome vary significantly from the regional trend underlining mechanical decoupling of the lower crust from the rest of the lithosphere. These differences diminish if cooler temperatures and, hence, stronger rheologies are considered. Lithospheric strength also exerts a profound control on the basin architecture and the surface expressions of extension, i.e., rift flank uplift and basin subsidence. If the lower crust is sufficiently weak, its flow towards the region of extended upper crust can provide a threshold value for the maximum subsidence which can be achieved during the syn-rift stage. In spite of continuous regional extension, corresponding burial history plots show exponentially decreasing subsidence rates which would traditionally be interpreted in terms of lithospheric cooling during the post-rift stage. The models provide templates to genetically link the surface and sub-surface expressions of lithospheric extension, for which usually no contemporaneous observations are possible. In particular, they help to decipher the information on the physical state of the lithosphere at the time of extension which is stored in the architecture and subsidence record of sedimentary basins.

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1. Introduction

Subsidence and sedimentary basin formation as well as uplift of fault-bounded rift shoulders are typical features of extended continental terrains like the East African rift system and the Basin and Range province (e.g., Coward et al., 1987; Cloetingh et al., 1998; Morley, 1999). While these vertical deflections of the earth’s surface can be easily monitored, the contemporaneous expressions of lithospheric extension in the subsurface are much more ambiguous. The distribution of stress and strain may be known locally from...
borehole data down to a few kilometres depth, but the deeper parts of the crust and the mantle lithosphere remain inaccessible for direct probing and information can only be gathered from earthquake analysis and geophysical imaging. These depth intervals only become accessible for geological studies if exhumation, i.e., due to continued extension and erosion or during subsequent continental collision, exposes them at surface. In these cases, however, the related surface expressions of lithospheric extension have long been destroyed by erosion.

A valuable tool which can help to genetically link the observations made at different crustal levels and to understand the spatial and temporal variations of stress and strain during lithospheric extension are numerical simulations. Such models use a quantitative description of the first-order physical processes acting in the lithosphere to calculate rock deformation on the basis of thermal and mechanical properties. Numerical simulations of continental extension have been presented in a number of papers which differ mainly in the methodology and model geometry used. Lithosphere-scale models without any predefined faults have been presented, for example, by Bassi (1991) and Hopper and Buck (1996). Other authors have used models with predefined zones of weakness which focus on the upper crust (Bott, 1997), on foot wall deformation (Wdowinski and Axen, 1992), the strong part of the lithosphere (Boutilier and Keen, 1994) and the entire lithosphere (Dunbar and Sawyer, 1988). More recently, lithosphere-scale models with self-localizing faults have been used to study the effects of surface processes on the style of lithospheric extension (Burov and Poliakov, 2001).

The present study focuses on the different expressions of extension at the various lithospheric levels. In particular, it tries to relates lithospheric deformation observed at surface, i.e., uplift and subsidence, to contemporaneous deformation in the deeper parts of the lithosphere. The study uses a model geometry which describes the mechanically strong part of the lithosphere and incorporates a pre-existing fault in the upper crust to represent older tectonic elements which then become reactivated in the extensional regime. Special focus is on strain partitioning within the rheologically layered lithosphere and local reorientations of the regional stress field.

2. Modelling approach

Numerical simulations are based on the finite element (FE) method as this technique allows the calculation of stresses, strains and temperatures in compositionally heterogeneous models with non-linear rheologies and complex geometries. Calculations are based on two-dimensional model geometries which represent a vertical cross-section through the upper lithosphere and include a pre-defined mechanical discontinuity in the upper crust, i.e., a pre-existing fault. Thermal modelling is based on heat transport by conduction and advection, while the mechanical simulations combine various material laws, e.g., brittle failure and temperature- and strain rate-dependent creep, to approximate the rheology of the lithosphere. A detailed description of the various modelling aspects can be found in the Appendix. Thermal and mechanical calculations are coupled using the finite element software package ANSYS® (Ansys Inc., Houston, USA).

2.1. Initial model geometry

The model describes a 200 km long section through the upper part of typical continental lithosphere extending from the Earth’s surface down to a depth of 58 km (Fig. 1). Upper and lower crustal thicknesses are 16 and 21 km, respectively. A 21 km thick piece of the upper mantle represents the mechanically strong part of the mantle lithosphere. The thermal and mechanical properties applied to these three model layers are summarised in Table. 1. The lowermost part of the mantle lithosphere contributes little to the overall strength of the continental lithosphere and is therefore not considered.

The upper crust contains a pre-defined fault surface dipping at 32° and extending down to the top of the lower crust at a depth of 16 km. The fault continues horizontally to the right side of the model. The fault geometry is designed to describe a former thrust which is reactivated during extension. Such an extensional reactivation of older compression-related structures is a common feature, e.g. during late-orogenic extension (collapse) or if rifting starts in the area of a former orogen. The model is subdivided into 1660 triangular and rectangular elements, whereas 2000 contact elements define the pre-existing fault.

2.2. Boundary conditions

Boundary conditions for the thermal calculations are a constant surface temperature of 0 °C and no lateral heat flow through the sides of the model. A constant basal heat flow was chosen as the lower boundary condition. In the different scenarios outline below its
value is varied between 10 and 26 mW m$^{-2}$ to study the impact of different crustal and lithospheric temperatures and, hence, strength on extension style.

Mechanical boundary conditions permit only vertical movements and no tilt, respectively, at the sidewalls of the model. Isostatic forces act on the base of the model, while the top is essentially a free surface. Only in those parts where the basement subsides below a certain reference level, a pressure equivalent to the load effect of the sedimentary basin fill acts on top of the model. In order to simulate extension or compression either displacements or forces can be applied to the sides of the model. In the present model, the left wall is fixed horizontally while the right side is moved at a constant velocity of either 0.2, 2 or 20 mm a$^{-1}$ to simulate horizontal extension.

3. Model scenarios

In principle, the numerical approach would allow to study systematically the impact of all input parameters as well of the initial and boundary conditions once the model geometry has been set up. However, such an encyclopaedic parameter analysis would go far beyond the scope of this paper. Instead, work concentrates on the two most important parameters influencing the modelling results which are temperature and strain rate. Due to the strong temperature-dependence of the creep laws and the depth of the brittle–ductile transition, temperature has a profound control on the style of lithospheric extension. Three numerical experiments differing in the initial temperature distribution and, hence, strength of the continental lithosphere are studied in detail. The scenarios intend to represent a mechanically weak, moderately strong and strong lithosphere. These differences in strength are achieved by varying the basal heat flow and consequently the initial lithospheric temperatures. The extension velocity in all three cases is 2 mm a$^{-1}$. Two further scenarios address the effect of different strain rates on lithospheric deformation. Strain rates influence the modelling results not only because of the strain-rate dependence of the creep laws but also through their impact on heat advection.

3.1. Scenario I: Extension of ‘hot’ (low strength) continental lithosphere

The first scenario examines extension of a comparatively hot continental lithosphere with a basal heat flow of 26 mW m$^{-2}$ and a Moho temperature of 810 °C. Such high temperatures can occur, for example, in active rift settings above an ascending mantle plume and during advanced stages of lithospheric

![Fig. 1. Initial finite element grid (top), material distribution (centre) and temperature field (bottom) of the two-dimensional half-graben model. The initial dip of the fault is 32°. Temperatures shown are for scenario II which represents a “warm” (medium strength) continental lithosphere. The tensile strength profile through the model lithosphere is calculated for a strain rate of 1 × 10$^{-15}$ s$^{-1}$.](image)
extension and asthenospheric upwelling by passive rift mechanisms, respectively. The high temperatures pronounce the rheological contrasts between the various lithospheric units and result in a particularly low strength of the lower crust. Some of the modelling results for this scenario, i.e., deformed FE grids, horizontal and vertical displacements as well as strain distributions, are shown in Figs. 2 and 3. They represent two evolutionary stages after 16 and 28 km of lithospheric stretching, i.e., 8 and 14 Myr after the onset of extension.

### 3.2. General observations

Modelling depicts two prominent features which are both genetically linked to the pre-defined fault: a 5 km deep half-graben and a dome-shaped uplift of the lower crust beneath the sedimentary basin. Thus, the lower crust is thickest where upper crustal thinning reaches its maximum. A detailed inspection of the model geometry after 28 km extension (Fig. 3) shows that beneath the half-graben the upper crustal basement has been thinned to less than 6 km thickness, which is equivalent

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#### Thermal lithosphere properties

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<td>Upper crust</td>
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| Thermal conductivity, W m⁻¹ °C⁻¹ | k | 3 – 1.3 | Zoth and Hanel (1988)
| Specific heat, m² s⁻² °C⁻¹ | C | 1.3 × 10³ |
| Radiogenic heat production, W m⁻³ | H | 2.3 × 10⁻⁶ |
| Lower crust | | | |
| Thermal conductivity, W m⁻¹ °C⁻¹ | k | 2.5 – 1.7 | Zoth and Hanel (1988)
| Specific heat, m² s⁻² °C⁻¹ | C | 1.3 × 10³ |
| Radiogenic heat production, W m⁻³ | H | 0.5 × 10⁻⁶ |
| Upper mantle | | | |
| Thermal conductivity, W m⁻¹ °C⁻¹ | k | 3 – 4 | Zoth and Hanel (1988)
| Specific heat, m² s⁻² °C⁻¹ | C | 1.3 × 10³ |
| Radiogenic heat production, W m⁻³ | H | 0.02 × 10⁻⁶ |

#### Mechanical lithosphere properties

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* Value is temperature-dependent.
to a local stretching factor of 2.7. In contrast, the lower crust in this area has achieved a thickness of 20.5 km compared to 19 km in other parts of the model. Regarding the initial lower crustal thickness of 21 km this is equivalent to a stretching factor of 1.11, while it is close to 1.0 in the area of the lower crustal dome. As a consequence of this differential, but counteractive deformation in upper and lower crust the Moho shows no major relief but only a gentle upwarp slightly offset (15 km) with respect to the basin centre. The strong part of the mantle lithosphere shows a thickness between 17 and 19.5 km and stretching factors ranging between 1.24 and 1.08. With respect to the initial length of the entire model section, 28 km of extension correspond to an average stretching factor of 1.14.

Lithospheric extension and the related dome-shaped uplift of the lower crust have also led to an anti-clockwise rotation of the predefined normal fault. Its dip has decreased from initially 32° to 20° (Fig. 3a). The central part of the normal fault has a convex-upward shape.

3.3. Displacement of the model surface

Horizontal extension also results in vertical displacement of the model surface, which can be compared to
uplift and subsidence patterns observed at the earth’s surface. Uplift occurs in the footwall immediately next to the pre-defined fault. After 8 Myr and 16 km of extension, respectively, the rift shoulder stands up to 1.2 km above the surrounding topography (Fig. 4; no erosion case), while the basin has subsided 4 km. After 14 Myr and 28 km of extension, maximum subsidence in the half-graben has reached about 5 km. The temporal evolution of subsidence at the basin’s depocentre can also be expressed in form of the commonly used burial history plots which display time after the onset of extension vs. subsidence (Fig. 5). For the “hot” scenario, it shows that subsidence rates are fairly constant during the first rifting stage. After about 5 Myr subsidence rates progressively slow down and finally approach very low values.

3.4. Strain distribution

Figs. 2d and 3d illustrate how differently extensional strain is partitioned between the various lithospheric units. In the upper crust, differential movements between foot wall and hanging-wall concentrate on the predefined fault. No reactivation and differential movements occur along the horizontal segment of the predefined fault as fault strength is higher than the strength of the lowermost upper crust. Thus, it is mechanically more feasible to form a new ductile shear zone in the
lowermost crust than to overcome the frictional resistance of the old existing fault. A small depression in the hanging wall also showing up on the strain plots (Figs. 2d and 6d) as a V-shaped contour pattern points towards the formation of a secondary basin structure, a so-called crestal collapse graben.

In the lower crust the strain distribution is highly variable. Maximum deformation is achieved in a narrow zone where the fault projects into the lower crust. In the mantle lithosphere deformation is essentially distributed over the whole model width showing only a weak maximum in the area where the high-strain zone in the lower crust reaches the Moho. These strain patterns result from the interaction of the pre-defined fault with the rheologically layered lithosphere. High strain zones occur where weak rheologies are located next to strong rheologies, i.e., at the base of the upper and the lower crust, particularly in the vicinity of the lower crustal dome. The prominent high strain zone cutting through the lower crust is genetically related to the upper crustal fault. Although discrete fault movements are restricted to the upper crust the fault also acts as a stress guide projecting into the lower crust.

Fig. 4. Topography of the model surface after 16 km of extension for all three scenarios studied (15 × vertical exaggeration). Curves represent uplift and subsidence of the earth’s surface and top of the pre-rift basement (in the area of the sedimentary basin), respectively, relative to their initial positions.

Fig. 5. Burial history of the sedimentary basin for all three scenarios studied. Curves show subsidence vs. time and amount of extension, respectively, for the point of maximum vertical displacement, i.e., the tip of the hanging wall.
The strain distribution in the lower crustal dome beneath the sedimentary basin is variable. The core of the dome shows surprisingly little deformation. Although it is the part of the lower crust which experiences the most vertical uplift (Figs. 2c and 3c), it is also the part which suffers the least deformation, i.e., less than 10%. Strain increases towards the flanks of the dome, particularly on the side which is affected by the predefined fault.

3.5. Stress distribution

The crustal and upper mantle stress fields in the vicinity of the sedimentary basin are shown in Fig. 6. The vectors indicate the orientation of the largest and least principal stress $\sigma_1$ and $\sigma_3$, and their lengths are proportional to the stress magnitudes. The displacement boundary condition selected for this scenario implies an overall orientation of $\sigma_3$ in horizontal direction. While this regional stress regime is found in parts of the crust and the entire mantle lithosphere, significant reorientations occur next to the fault and especially in the lower crustal dome. Variable stress field orientations in the upper crust occur in its lowermost, i.e., weakest part, next to the fault. The stress pattern in the lower crustal dome shows a progressive deviation from the regional trend towards the core. There the $\sigma_3$ directions are essentially vertical, whereas in the immediately overlying upper crust and underlying mantle they are oriented subhorizontally. This stress pattern further illustrates the strong mechanical decoupling of the lower crust from the rest of the lithosphere.

3.5.1. Scenario II: Extension of ‘warm’ (medium strength) continental lithosphere

This scenario differs from the previous experiment only in a lower heat flow, which in turn increases the initial strength of the lithosphere. The reduced basal heat flow of 19 mW m$^{-2}$ results in a Moho temperature of 636 °C. The consequences of this simple parameter variation are significant as the lower temperatures strongly reduce the rheological contrasts between the various lithospheric units (Fig. 7). For the same amount of stretching (16 km) as before, extension now results in formation of a 5.2 km deep half-graben, whereas it was 4.2 km in the “hot” scenario. The basin is also wider and the rift shoulder uplift lower (Fig. 4). In contrast, the lower crustal dome is less pronounced and the lower crustal thicknesses range between 19 and 20 km. Thus, the lower crust is extended more uniformly with a maximum in the prolongation of the shear zone while the minimum is located in the core of the lower crustal dome (Fig. 7d). A closer inspection of the deformed finite element grid reveals differential movements between upper and lower crust along the entire length of the predefined fault (Fig. 7a). In contrast to the “hot” scenario, the base of the upper crust now has an increased strength which makes it mechanically easier to reactivate the existing fault than to create a new shear zone in the lowermost crust. As a consequence the hanging wall block is moved homogeneously without much internal deformation except near its tip. High strain zones are restricted to the lowermost upper crust near the kink in the fault and its projection in the lower crust.

The higher strength and consequently lower mobility of the lower crust is also reflected in the subsidence...
history. Fig. 5 shows almost constant subsidence rates during the first 5 Myr of extension, then subsidence rates progressively slow down.

Stresses in the model lithosphere are much more uniform in orientation, particularly in the lower crustal dome reflecting the overall extensional setting, i.e., \( \sigma_3 \) oriented horizontally. Only in the immediate vicinity of the fault some stress field reorientations do occur.

3.5.2. Scenario III: Extension of ‘cold’ (high strength) continental lithosphere

The thermal boundary condition selected for this numerical experiment further amplifies the differences with respect to the “hot” scenario (Fig. 8). A basal heat flow of 10 mW m\(^{-2}\) results in a Moho temperature of 450 °C and largely minimizes the strength contrast between upper and lower crust and lower crust and mantle lithosphere, respectively. Isolines for horizontal and vertical displacement (Fig. 8b and c) illustrate that lower crust and mantle lithosphere are extended in a rather uniform manner. Likewise, strain is distributed more uniformly and lower crustal maxima and minima are much less pronounced than in the previous scenarios. In the upper crust higher strain occurs only near the fault kink and in the lowermost footwall beneath the fault zone. As a consequence,
neither the top of the lower crust nor the Moho shows any substantial relief. The entire hanging wall has moved in an en-bloc manner the full prescribed amount of extension resulting in large differential displacements between upper and lower crust across the fault zone.

After 16 km of extension, a 6.5 km deep and 50 km wide sedimentary basin has formed—deeper and broader than in the previous scenarios. Its asymmetric, half-graben geometry is fostered by very little lower crustal doming and minimal fault rotation. Rift shoulder uplift is more local and reaches only 0.15 km (Fig. 4). The subsidence history (Fig. 5) shows the typical characteristics of the syn-rift stage, i.e., constant rates throughout most of the model run. Only after about 8.5 Myr subsidence rates start to slow down.

Stresses in the model lithosphere are uniform in orientation throughout with a horizontal $\sigma_3$ orientation everywhere.

3.5.3. Scenario IV: Slow extension

This scenario studies the effect of lower strain rates on the modelling results. The extension velocity is

![Diagram](image_url)
0.2 mm a\(^{-1}\), i.e., an order of magnitude slower than in the previous cases. The initial temperature distribution is identical to scenario II representing a ‘warm’ (medium strength) continental lithosphere.

Because of the very slow extension rates, thermal equilibration by heat conduction can easily keep pace with heat advection. Thus, the temperature field throughout the simulation is characterized by slowly decreasing temperatures due to thinning of the radiogenic heat producing layers and subhorizontal isotherms, respectively. The strain distribution (Fig. 9a) shows in large parts of the model a pronounced high-strain zone near the base of the upper crust. The deformation pattern in the lower crust and upper mantle lithosphere is almost symmetrical and shows two areas of enhanced strain dipping towards the left and right side of the model. They originate at the crest of the lower crustal uplift. If compared to the results of scenario II, there is no localized higher strain zone in the lower crust, but a distinct area of higher deformation at the base of the upper crust in the hanging wall which is missing in Fig. 7d.

3.5.4. Scenario V: Fast extension

This scenario is intended to study the effect of high strain rates on lithospheric deformation. The extension velocity is 20 mm a\(^{-1}\), i.e., similar to plate velocities and 10 times faster than in the first three cases. Again, the temperature distribution of scenario II is adopted.

In contrast to the previous scenario, heat transport by advection plays a profound role. As basin formation is very rapid (e.g., 16 km of extension in 0.8 Ma), thermal equilibration by heat conduction is much slower than heat advection. Consequently, temperatures in the lithosphere model hardly change throughout the simulation. The strain distribution (Fig. 9b) in the upper crust shows a high-strain zone in the hanging wall resembling an antithetic fault, but no enhanced deformation at its base. Deformation in the lower crust and upper mantle lithosphere is asymmetrical with larger deformation in the right half of the model. Maximum straining occurs in the lower crust in continuation of the prescribed normal fault. Altogether, this strain pattern more resembles scenario III which is characterized by both lower temperatures and lower strain rates.

With respect to surface topography and basin geometry, the footwall uplift is more pronounced in the slow extension case, while the basin is about 900 m deeper in the fast extension scenario. Consequently, lower crustal doming and uplift of the lower crust is larger in scenario IV.

A comparison of the effective forces required to maintain the prescribed constant velocity boundary condition is given in Fig. 10. It shows the vertically integrated deviatoric stresses at the left and right model boundary for extension rates of 0.2, 2 and 20 mm a\(^{-1}\). While the effective forces for the two faster scenarios show only relatively small variations with time, in the very slow case there is a significant
increase in the integrated deviatoric stress with progressive extension.

4. Discussion and conclusions

The modeling study shows that already for simple geodynamic boundary conditions the interference of the pre-existing fault with the rheologically stratified lithosphere can result in stress and strain patterns which differ substantially in space and time. This holds in particular for the “hot” – and less pronounced also for the “warm” – lithosphere model in which the lower crust is substantially weakened. Due to its low effective viscosity the lower crust can flow according to lateral pressure gradients (e.g., Block and Royden, 1990; Hopper and Buck, 1996). This flow is directed towards the lowest lithostatic pressure acting on the lower crust which in turn coincides with the maximum of upper crustal thinning. The lower crust is thus able to maintain a kind of intracrustal isostatic balance and can compensate laterally varying degrees of upper crustal thinning achieving a subhorizontal Moho relief (Wernicke, 1990). The inward directed lower crustal flow thickens the lower crust beneath the basin relative to the surrounding, thus, forming a dome-shaped uplift of lower crustal rocks. The strain pattern indicates that the core of the dome experiences only minor deformation, but is the part of the lower crust which is exhumed and decompressed the most. The lithosphere geometry depicted in Fig. 3a with this lower crustal dome can be considered also as an early stage in the evolution of metamorphic core complexes. If extension continues the normal fault will rotate further and the upper crust will be progressively thinned out until ultimately the lower crustal dome will reach the surface (Wernicke and Axen, 1988; Wdowinski and Axen, 1992). Metamorphic core complexes now exposed at surface document this inward directed flow indicated by the models. In the Ruby Mountains core complex (MacCready et al., 1997), for example, the large-scale folding and stretching lineation pattern demonstrate material transport towards the core itself.

Modelling results also show that the stress fields in this lower crustal dome differ in magnitude and orientation significantly from the regional trend which underlines mechanical decoupling of the lower crust. Thus, if lower crustal rocks are exposed at surface and are studied using traditional structural mapping techniques, a highly variable orientation of the stress field may be difficult to interpret in spite of the simple overall geodynamic scenario. Commonly such close spatial variations would be interpreted in terms of multiple tectonic episodes or short-term fluctuations of the regional stress field, but the numerical simulation show that substantial local stress perturbations can result even for very simple tectonic scenarios.

Fault geometry and lithospheric rheology also have a profound control on sedimentary basin architecture, subsidence history during the synrift stage and surface topography in the vicinity of the master fault. A low strength of the lower crust promotes a rather symmetric basin geometry in spite of the asymmetric model geometry with one normal fault only. In contrast, the cooler and stronger models result in a typical asymmet-

Fig. 10. Evolution of the vertically integrated deviatoric stress with time for three different extension velocities (right model boundary=filled boxes, left model boundary open circles).
ric basin architecture with a half-graben geometry. Another surface expression of crustal extension and consequently a common morphologic feature of extended terrains is the uplift of the rift shoulder, i.e., the footwall next to the fault. It results from unloading of the foot wall and flexural rotation of the normal fault (Buck, 1988). In case of the high-strength models this rift shoulder uplift is minimal, whereas in the “hot” scenario substantial uplift occurs. In this case, counter-clockwise fault rotation is maximal and facilitated by lower crustal doming.

Another interesting outcome of the numerical simulations is that as inward lower crustal flow can partly compensate upper crustal thinning it provides a threshold value for the maximum subsidence which can be achieved during the initial rifting stage. The value depends mainly on temperature, i.e., it is larger for cooler rifted crust. Such a threshold value for subsidence has already proposed by Bott (1997), but for different reasons. Corresponding burial history plots show exponentially decreasing subsidence rate already during the syn-rift stage, although regional extension continues at an unchanged speed. Such subsidence curves would commonly be interpreted in terms of reduced extension rates or even the transition from syn- to post-rift (thermal) subsidence after active tectonic extension has ceased. It can be shown that the inward flow of lower crustal rocks progressively compensates the subsidence due to upper crustal thinning, thus limiting the maximum subsidence to about 5 km in case of the ‘hot’ scenario. For cooler temperatures, the higher strength of the lower crust impedes differential thinning and large-scale flow towards the minimum lithostatic pressure beneath the sedimentary basin. The corresponding subsidence histories illustrate the reduced capability of the lower crust to counteract upper crustal thinning by inward directed lower crustal flow, hence resulting in deeper basins and more uniform subsidence rates during the syn-rift stage.

If compared to temperature, the effect of strain rate on lithospheric deformation is more subtle and more difficult to predict as there is a trade-off between the temperature-and the strain rate-dependent effects of rock deformation and the thermal structure, respectively. Higher strain rates increase the strength in the ductile regime, but this can be counteracted by heat advection which – if compared to slower extension – maintains relatively higher temperatures and, hence, reduces rock strengths. In contrast, low strain rates will weaken the rock, but as thermal equilibration by conduction is dominant, the lower temperatures will in turn lead to higher strengths. The different extension velocities in scenarios II, IV and V clearly lead to different deformation patterns for a given thermal and lithosphere structure, but any application to field example will require a careful analysis of the local thermal material parameters and creep laws.

In summary, the modeling study illustrates that even a very simple tectonic scenario, i.e., wholesale lithospheric extension at a constant velocity, can result in a highly variable stress and strain distribution in the lithosphere. Further variations will result if more complex model geometries (material heterogeneities, multiple faults) and multiple rifting episodes are considered. With respect to basin formation, basin geometry as well as the subsidence history vary substantially with the physical state of the lithosphere. This holds particularly for conditions which maximize the rheological contrasts between the individual layers of the lithosphere, i.e., if high temperatures and/or appropriate creep laws result in a particularly low strength of the lower crust. Such conditions foster a mechanical decoupling of the lower crust from the upper crust and uppermost mantle lithosphere, respectively. The differences successively diminish for lower temperatures which increase particularly the strength of the lower crust and lead to a more uniform mechanical response of the entire lithosphere. The physical state of the lithosphere is not only documented in the deeper parts of the crust but also basin shape, shoulder uplift and subsidence history reflect the rheology and, hence, temperature distribution of the extended lithosphere. Thermomechanical models can be a valuable tool to decipher this record and improve our understanding of lithospheric deformation and sedimentary basin formation.

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Appendix A

The finite element models are based on coupled thermal and mechanical calculations and use contact elements to describe pre-existing zones of weakness, i.e., faults.

A.1. Thermal calculations

The thermal calculations are based on heat transport by conduction and advection. Among others, the lithospheric temperature field depends on material properties
like thermal diffusivity and the internal heat production due to the decay of radioactive elements. The governing equation (e.g., Carslaw and Jaeger, 1959) is

\[
\rho \cdot c \cdot \left( \frac{\partial T}{\partial t} + v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} + v_z \frac{\partial T}{\partial z} \right) = \kappa \frac{\partial^2 T}{\partial x^2} + \kappa \frac{\partial^2 T}{\partial y^2} + \kappa \frac{\partial^2 T}{\partial z^2} + A
\]

(1)

where \( \rho \) is density, \( C \) is specific heat, \( \kappa \) is thermal diffusivity (=thermal conductivity \( k/\rho \cdot C \)) and \( A \) is radiogenic heat production. \( v_x \) and \( v_y \) describe displacement in the coordinate directions \( x \) and \( y \), whereas \( T \) is temperature and \( t \) is time. However, some of the material parameters themselves depend on temperature. Density, for example, decreases with increasing temperature. A similar temperature-dependence holds for thermal conductivity. Within the range of upper lithospheric temperatures, thermal conductivity of most rocks decreases with temperature. The exact relationship depends mainly on mineral composition, porosity and pore fill (e.g., Clauser and Huenges, 1995). Zoth and Hänel (1988) propose that thermal conductivity \( k(T) \) is a function of temperature \( T \) according to

\[
k(T) = A + \frac{B}{350 + T}
\]

(2)

where \( A \) and \( B \) are empirical constants depending on the rock type. Their data for felsic (\( A=0.64, B=807 \)) and mafic rocks (\( A=1.18, B=474 \)) are used to represent the temperature-dependent thermal conductivities in upper and lower crust, respectively. Thus, thermal conductivities range between 1.5 and 3 W m\(^{-1}\) K\(^{-1}\) within most parts of the crust. For the thermal conductivity of the mantle lithosphere a relationship given by Buntebarth (1980) is used. It shows that at temperatures above 500 °C the thermal conductivity of peridotites increases slowly with increasing upper mantle temperatures. However, the exact relationship strongly depends on the fayalite–forsterite ratio in the olivine (e.g., Clauser and Huenges, 1995).

### A.2. Mechanical calculations

The mechanical behaviour of the lithosphere can be characterized by various rheological laws which depend mainly on rock composition, temperature, pressure, strain and strain rate (e.g., Ranalli, 1995). The most important deformation mechanisms are elasticity, brittle failure and viscous flow. Elasticity is used to describe the recoverable strains of model materials at low differential stresses, but is restricted to a few percent of deformation only. Brittle deformation by fracture and frictional sliding on existing faults occurs if the applied stress exceeds the brittle strength. Brittle strength can be estimated according to the Coulomb-Navier criterion (e.g., Jaeger and Cook, 1979; Ranalli, 1995) which gives the critical shear stress \( \tau_{\text{crit}} \) required to overcome frictional resistance by

\[
\tau_{\text{crit}} = C + \mu \cdot \sigma_n \cdot (1 - \lambda)
\]

(3)

where \( C \) is cohesion, \( \mu \) is coefficient of friction, \( \sigma_n \) is normal stress and \( \lambda \) is the ratio of pore pressure to lithostatic pressure. Byerlee (1978) empirically found the following material parameters for \( C \) and \( \mu \) which are largely insensitive to rock type and temperature:

\[
\begin{align*}
C &= 0 \text{ MPa}, & \mu &= 0.85 & \text{ for } (1 - \lambda)\sigma_n & \leq 200 \text{ MPa} \\
C &= 60 \text{ MPa}, & \mu &= 0.6 & \text{ for } (1 - \lambda)\sigma_n & \geq 200 \text{ MPa}.
\end{align*}
\]

Several authors (e.g., Carter and Tsen, 1987; Kohlstedt et al., 1995) emphasize that these material constants are valid only for the upper crust and already provide an upper limit for the actual strength below depths of 5 km. If one of the principal stresses coincides with the vertical stress as is the case close to the earth’s surface, Eq. (3) can be recast in terms of the differential stress \( \sigma_1 - \sigma_3 \) as

\[
\sigma_1 - \sigma_3 = A \cdot g \cdot \rho \cdot z(1 - \lambda).
\]

(4)

(Bibson, 1977; Ranalli, 1995), where \( g \) is gravitational acceleration, \( \rho \) is the density of the rocks overlying a depth \( z \) and \( A \) is a parameter that depends on the coefficient of friction and the predominant type of faulting. This approach assumes that the orientation of the pre-existing faults is that given by frictional theory and that cohesion on the faults is negligible when compared with effective normal stress. Assuming no cohesion and a coefficient of friction of 0.85 as is suggested by Byerlee (1978) for the uppermost crust, values for \( A \) of 3.7 and 0.78 can be adopted for thrust and normal faulting, respectively. Thus, for frictional sliding on normal faults assuming a hydrostatic pore-fluid pressure (\( \lambda = 0.36 \)) and an average density of 2750 kg m\(^{-3}\), Eq. (4) results in a tensile strength gradient of about 14 MPa km\(^{-1}\). In the finite element model, brittle behaviour is approximated by continuum deformation using an elastic – perfectly plastic flow law with a depth – (vertical stress-) dependent yield stress. Thus, material behaves elastically at stresses below the yield stress as defined by Eqs. (3) and (4), but flows instantaneously according to an ideal plastic flow law if the yield stress is exceeded. This rheology is designed to account for permanent strain at stress levels above the yield stress, but does not explicitly describe frictional sliding and fault movement.
As temperature increases with depth, ductile flow becomes important and lithospheric deformation is assumed to be governed by thermally activated power law dislocation creep. The non-linear relationship between strain rate \( \dot{e} \), differential stress \( \sigma_1 - \sigma_3 \) and temperature \( T \) is given by

\[
\sigma_1 - \sigma_3 = \left( \frac{\dot{e}}{A} \right)^{1/n} e^{Q/(nRT)}
\]

where \( R \) is the universal gas constant and \( a_0 \) (strain rate coefficient), \( n \) (power law stress exponent) and \( Q \) (activation energy) are material properties derived from laboratory experiments (e.g., Ranalli, 1995). Power law creep holds for high temperatures and low to moderate differential stresses. At low temperatures or high stresses, this relation vanishes and strength becomes rather independent of strain rate and temperature (Carter and Tsen, 1987).

The rheological laws outlined above are combined to calculate lithospheric strength in the mechanical model. The specific strength at any given point in the lithosphere is determined either by the modified Coulomb-Navier criterion (Eqs. (3) and (4)) or by power law dislocation creep (Eq. (5)) depending on which deformation mechanism provides the lowest yield strength. The rheological law for each element is not fixed but is continuously updated depending on the actual temperature, pressure, strain and strain rate.

The rheological stratification of the continental lithosphere is modelled using the power law creep parameters of wet quartzite, anorthosite and wet dunite for the upper crust, lower crust and mantle lithosphere, respectively (Paterson and Luan, 1990; Shelton and Tullis, 1981; Chopra and Paterson, 1981). These creep parameters do not intend to imply a corresponding monomineralic composition of the lithosphere. They rather approximate the rheology of the weakest interconnected phase which determines the actual strength of the rock in each of the three layers (Handy, 1990). At the present stage of knowledge, these rheological laws can give only approximate descriptions of the true lithospheric deformation at geological strain rates. The uncertainties result not only from the little known physical and chemical heterogeneities of the lithosphere, but are also caused by extrapolation of rheologies measured at experimental conditions several orders of magnitudes faster than geological strain rates (see Kohlstedt et al., 1995 for a comprehensive discussion).

In summary, the rheology of the lithosphere is approximated by three different material types each capable of deforming with elastic, perfectly plastic or non-linear viscous behaviour. The top of the model is essentially a surface free of any mechanical boundary conditions. Only in those parts where the basement subsides below a certain reference level a vertical stress according to

\[
\sigma_{zz} = \rho_{sed} g z_{sub}
\]

is applied to account for the load effect of the sedimentary basin fill. In this formula, \( \rho_{sed} \) is the average sediment density, \( g \) is the gravitational constant and \( z_{sub} \) is the basement subsidence (relative to its initial position). At the base of the model so-called buoyancy rollers (e.g., Boutilier and Keen, 1994) are used to describe isostatic forces.

### A.3. Numerical description of pre-existing faults

Pre-existing zones of mechanical weakness and faults, respectively, can be incorporated in continuum models in various ways, e.g., using the slippery node technique of Melosh and Williams (1989) or a significantly finer numerical grid with reduced strength in the area of the fault (Boutilier and Keen, 1994). In this study so-called 2D point-to-surface contact elements are used to incorporate a mechanical heterogeneity and approximate a fault in the upper crust, respectively. This is an important extension of the continuum approach traditionally used in FE modelling as it allows to describe large differential movements between independently meshed parts of the model, i.e., between footwall and hanging wall blocks. Contact elements are defined at surfaces where model parts are in contact or may come into contact during the course of the numerical simulation. The element geometry is a triangle with two nodes on one of the surfaces (target nodes) while the third is located on the other surface (contact node). Contact elements can transmit stresses both normal and tangential to the contact surface. They are capable to consider friction on the contact surface as well as sliding deformation.

The properties of the contact surface can be controlled by the contact stiffness \( K \) and the coefficient of friction \( \mu \), among others. The contact stiffness \( K \) can be envisaged as the stiffness of a spring that is put between the two contacting areas when contact occurs. The amount of penetration between the two surfaces is therefore dependent on \( K \). Ideally, there should be no penetration, but this implies \( K = \infty \) and causes numerical convergence difficulties. Practically, the contact stiffness should be chosen so that the contact penetration is acceptably small but does not cause numerical problems. The contact stiffness ranges typically be-
between 0.1 and 10 times the elastic modulus of the contacting materials (see ANSYS® Structural Nonlinearities User Guide for further details).

The coefficient of friction \( \mu \) is a material property which—in case of a fault—depends on the contacting materials, surface roughness and the existence of smearing fault gauge and clay minerals, among others. Thus, the coefficient of friction can vary over a wide range, i.e., between 0.85, the typical value for intact rock and 0.18, if clay minerals are present (Meissner, 1986; Streit, 1997). For some faults, e.g., the San Andreas Fault in California, even lower friction coefficients down to 0.1 have been proposed (Lachenbruch and Sass, 1992). For the present modelling study, a moderate coefficient of friction of 0.4 is used.

A.4. Coupling of thermal and mechanical calculations

The rheology of crust and upper mantle strongly depends on the temperature distribution, which, in turn, changes during lithospheric deformation due to thermal relaxation by heat conduction and advection. This thermo-mechanical coupling is modelled with two geometrically identical finite element grids which are used to solve the thermal and mechanical equations successively. After the initial temperature distribution is determined and applied to the temperature-dependent rheologies in the mechanical model, the numerical simulation progresses by calculating lithospheric deformation during a specified time step. The displacements determined by the mechanical model are then applied as \( \nu_x \) and \( \nu_y \) (see Eq. (1)) to modify the geometry of the thermal grid and a new, transient temperature field is calculated. Actualised temperatures and thermal stresses related to temperature changes are fed back into the next mechanical step and so on. Thus, mechanical and thermal calculations are coupled via temperatures and thermal stresses resulting from thermal expansion and via displacements. Depending on deformation and the importance of advective heat transport, respectively, the thermal–mechanical coupling time may vary between 50 and 500 ka.

References


