

# What has Thermodynamics to offer to Geodynamic Modeling

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## General Abstract

### Multiscale Earth System Dynamics Group

Our group aims at a tight integration of results from multiple disciplines (field-geology, microstructure analysis, geophysics and chemistry) using a self-consistent thermodynamical framework as a unifying framework.

Our numerical approach tackles the problem from two sides: the equilibrium and non-equilibrium side of thermodynamics. We use the Gibbs Energy Minimisation algorithm `Perple_X` in order to determine the equilibrium properties of the materials we want to investigate. The results of these calculations are compiled in the database `PreMDB`. Through the use of the Gibbs Energy Minimisation we can easily obtain material properties that can not be measured in a laboratory.

Essentially all processes observed in nature are irreversible and dissipate energy. For those processes the energy equation has to be solved in addition to the usual mechanical equations used in crustal geodynamics. Otherwise feedback mechanisms like shear heating or chemical strain will go unaccounted for. We are not concerned with reproducing individual geometries of individual geological settings but to prove that the general patterns observed in the earth are manifestations of a fully coupled thermo-mechanical equation system.

## Scientific Abstract

In our calculations we encounter two different thermodynamic length scales each with its different associated time scales. At the level of small scale volume discretisation we assume local equilibrium at the large scale we assume non-equilibrium

### The Equilibrium Side:

**The Preliminary Reference Earth Material DataBase** (`PreMDB`) aims to provide modellers with a complete and easy access to fundamental material data for terrestrial rocks and minerals. Currently, `PreMDB` lists 47 major rock forming and wet minerals and 10 terrestrial rocks, representing a standard for marine sediments, upper and lower continental crusts [2, 3], oceanic crust and mantle. For each rock and mineral, 20 thermodynamic, thermal, elastic, seismic and mechanical properties are defined between 0.05-5 GPa and 400-1600K. Thermodynamic potential functions are used to calculate reversible material properties of rocks and minerals. These material properties are thermodynamically self consistent. Transport properties are also included, but they derive from laboratory experiments (Siert, 2007)

### The Non-Equilibrium Side:

**The Finite Element Code** (`ABAQUS`) is used for solving the large scale framework. We use variational principles for numerically solving the maximum rate of entropy production. We explicitly solve for the development of non-equilibrium dissipative structures. The code does not use self-localization formulations from classical Soil Mechanics (e.g. Mohr Coulomb) but solve for the localization phenomenon explicitly from calculating non-linear feedbacks.

The equilibrium material properties are obtained by minimizing the Gibbs Energy of a system of  $i$ -components. The molar Gibbs Energies are known through laboratory experiments (Holland, 1998). The various material properties are calculated as extensive parameter partial derivatives. As an example the elastic compliance tensor  $s_{ijkl}$  is given.

$$dG = -SdT + VdP + \mu_i dN_i \quad (1)$$

$$s_{ijkl} = -\frac{1}{V} \frac{\partial^2 G}{\partial \epsilon_{ij} \partial \epsilon_{kl}} \quad (2)$$

The Gibbs Energy is not suitable for deforming system. In order to account for the energy balance during mechanical deformation we must use the Helmholtz Energy  $F$ . We use the Maximum Entropy Production principle to calculate the changes in the Helmholtz Energy.

$$\dot{F} = \dot{U} - \dot{T}S \quad (3)$$

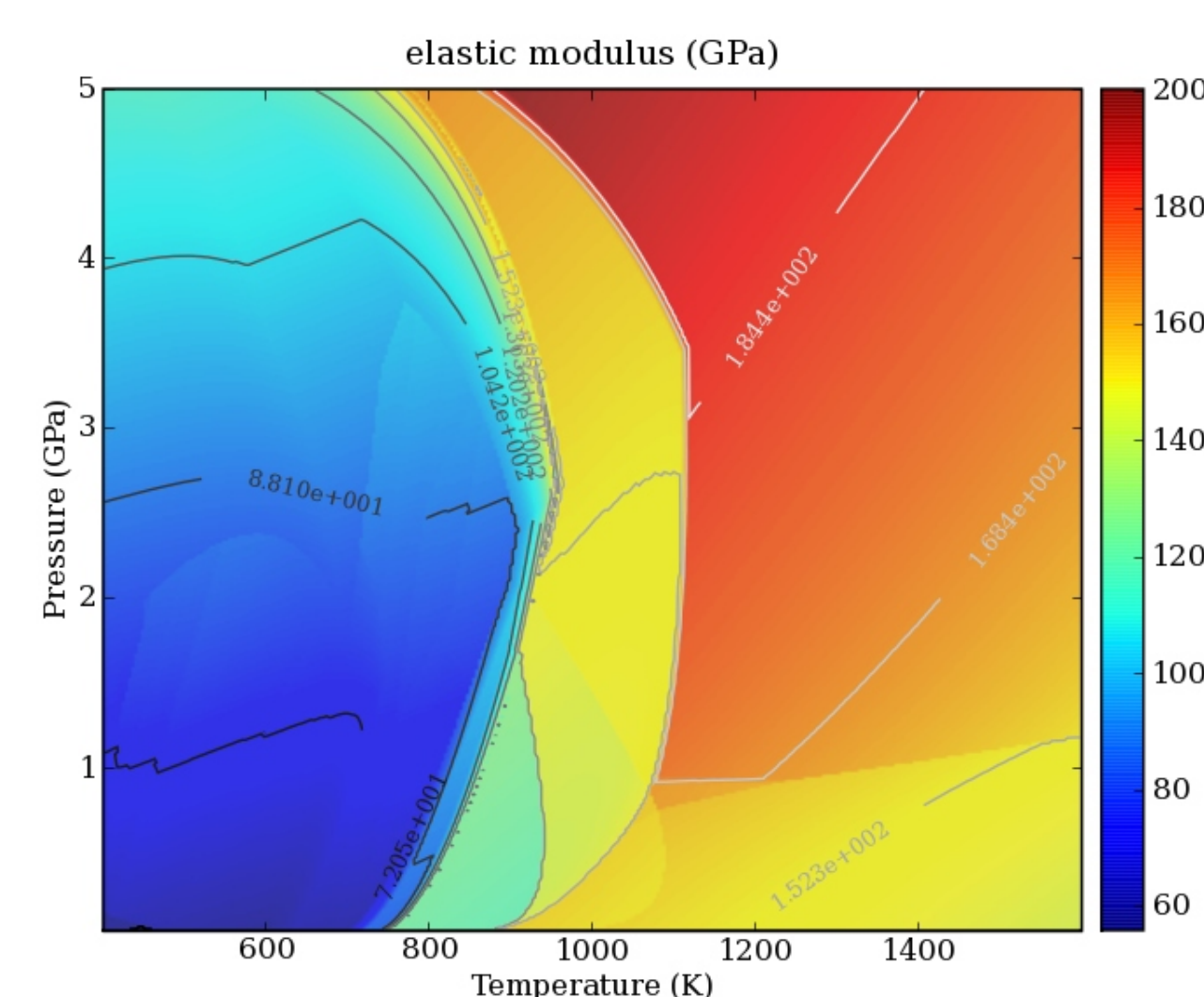
$$\Phi = \dot{T}S \rightarrow \max. \quad (4)$$

As an example we consider dissipation through shear heating.  $\chi$  gives the amount of deformation that is converted into heat. The second term (thermal expansion) and the third term (thermal diffusion) give further coupling to the mechanical deformation.

$$\rho c_p \frac{DT}{Dt} = \chi \sigma'_{ij} \epsilon'_{ij} + \lambda_{th} T_{equ} \frac{Dp}{Dt} - \rho c_p \kappa \nabla^2 T \quad (5)$$

## Equilibrium Material Data

The Field Observations provide constraints on Temperature and Pressure and the Chemical Composition needed to calculate the Equilibrium Material Data through Gibbs Energy Minimisation.

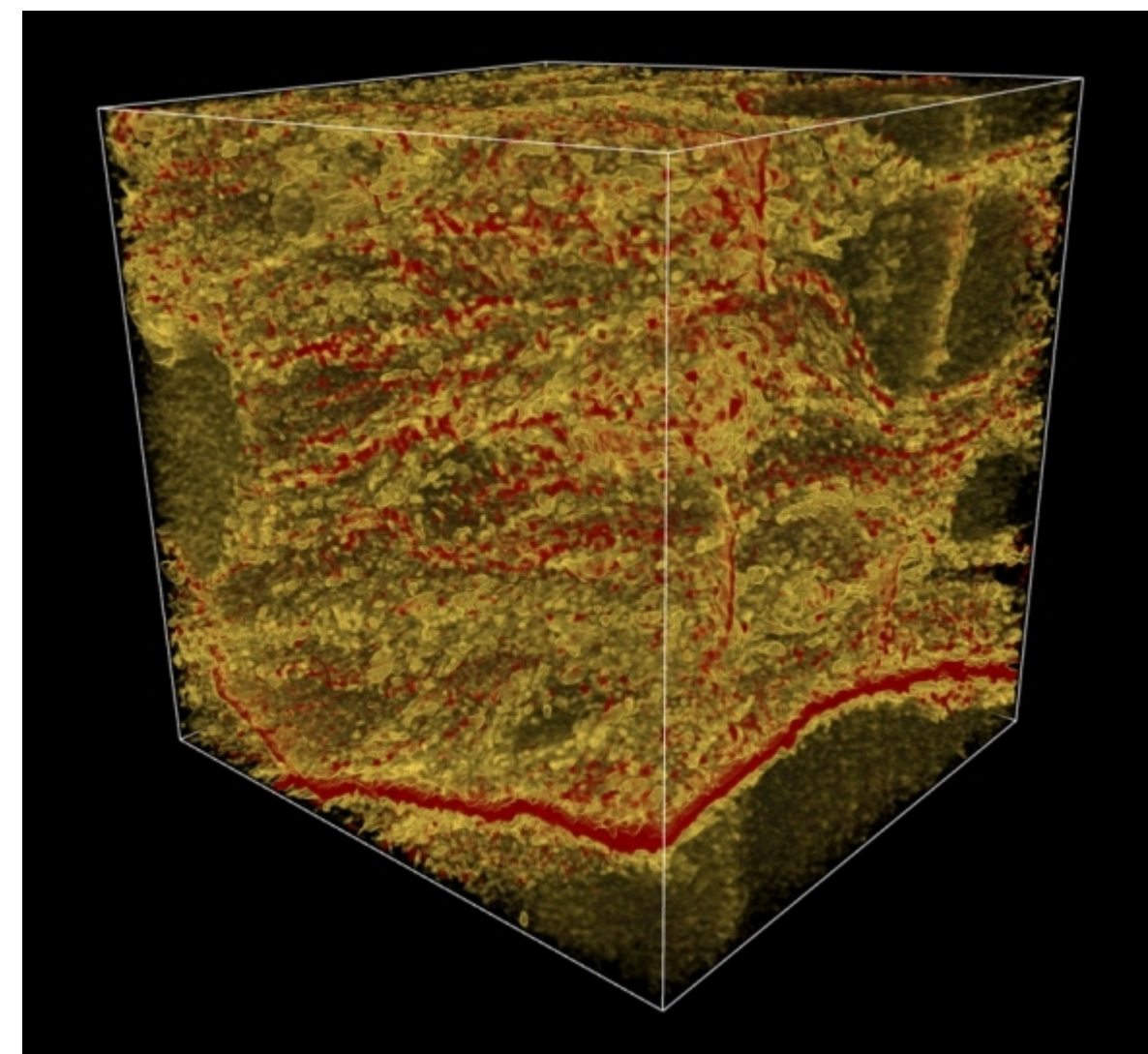


## Field Observation



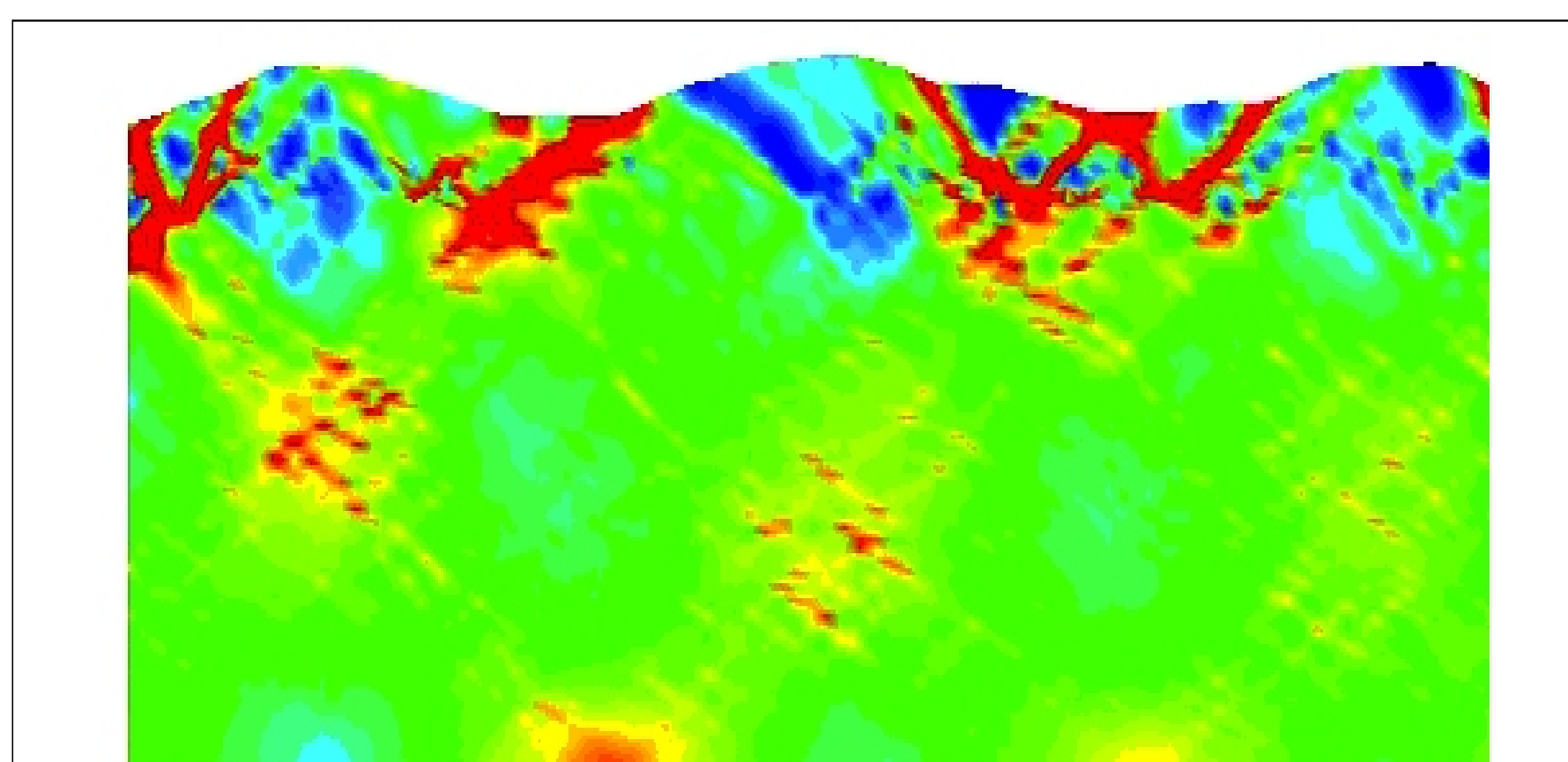
## Microstructural Analysis

The Microstructural Analysis gives us an estimation of the amount of energy that was dissipated in order to form new surfaces. It is also important for investigating the amount of chemical diffusion during deformation.



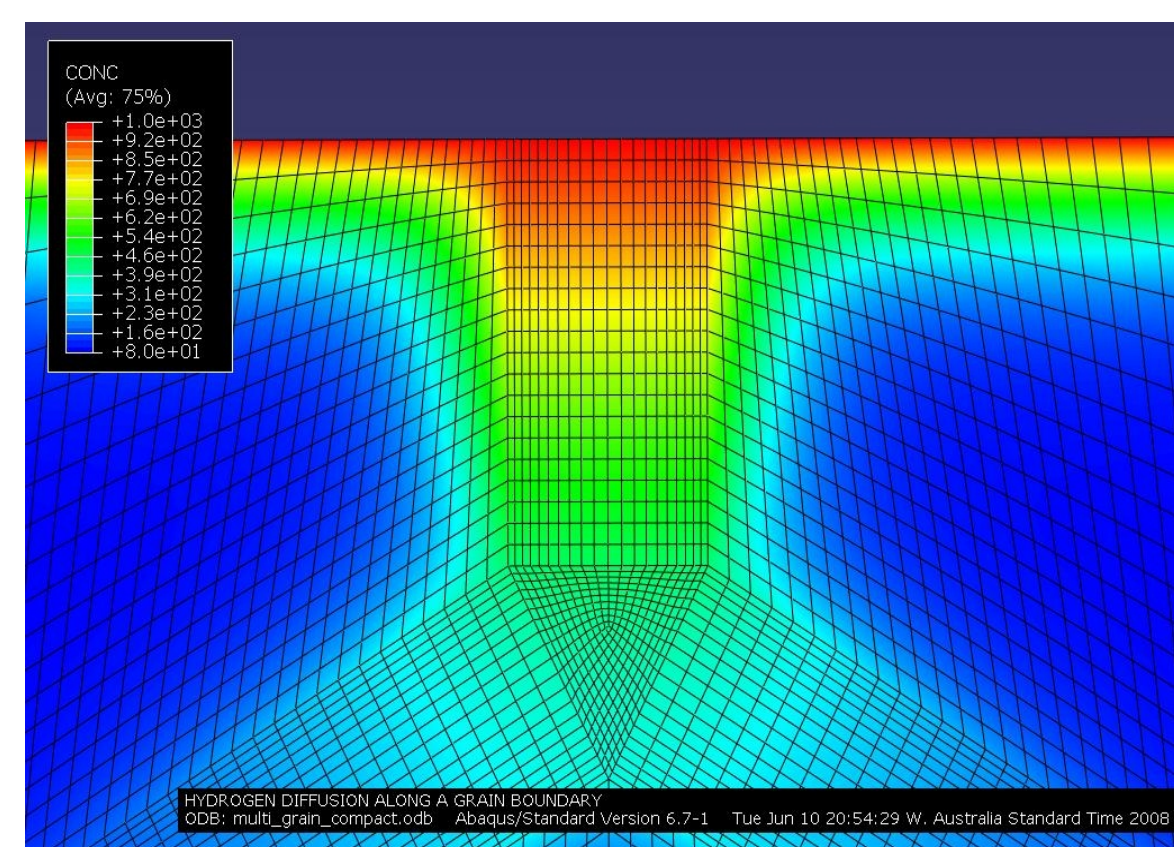
## Large Scale Simulation

A fully coupled simulation at a crustal scale was implemented successfully (Regenauer-Lieb, 2003). Thermomechanical coupling was considered and shear heating was used as the dissipative process.



## Grain Scale Simulations

Simulations at a grain scale become inevitable when we want to consider chemical-mechanical coupling which involves chemical diffusion processes and chemical strain. It is also important for grain size sensitive deformation mechanisms.



Questions we want to answer:

Why is there strain localisation?

How do flow laws and fracture strength depend on environmental parameters like water content?

Where is the switch between chemical diffusion and fluid flow?

## Glossary

### Fundamental Equation of Thermodynamics

Gives the Internal Energy  $U$  of a system as a function of the extensive parameters Entropy  $S$ , volume  $V$  and mole numbers  $N_i$

$$U = U(S, V, N_i)$$

The partial derivatives of the fundamental equation give the intensive parameters temperature  $T$ , pressure  $P$  and chemical potential  $\mu_i$

$$dU = TdS - PdV + \mu_i dN_i$$

### Helmholz Free Energy $F = U - TS$

$F$  is called "free" in analogy to the energy available to a heat engine for work. A heat engine drawing energy  $U = Q_1$  from a hot bath that must discharge an entropy  $S = Q_2/T_2$  into a cold bath can do work  $W = U - T_2 S$ .

### Gibbs Energy $G = U - TS + PV$

Systems at constant pressure and constant temperature minimize the Gibbs Energy. We use the derivatives of the Gibbs Energy to determine the equilibrium material properties in our models.

### Entropy & Dissipation

Entropy measures the irreversible changes in a system. It can be considered as the energy that is lost or dissipated in an irreversible process at a certain temperature. A system at equilibrium has maximized the entropy.

### Non-Equilibrium Thermodynamics

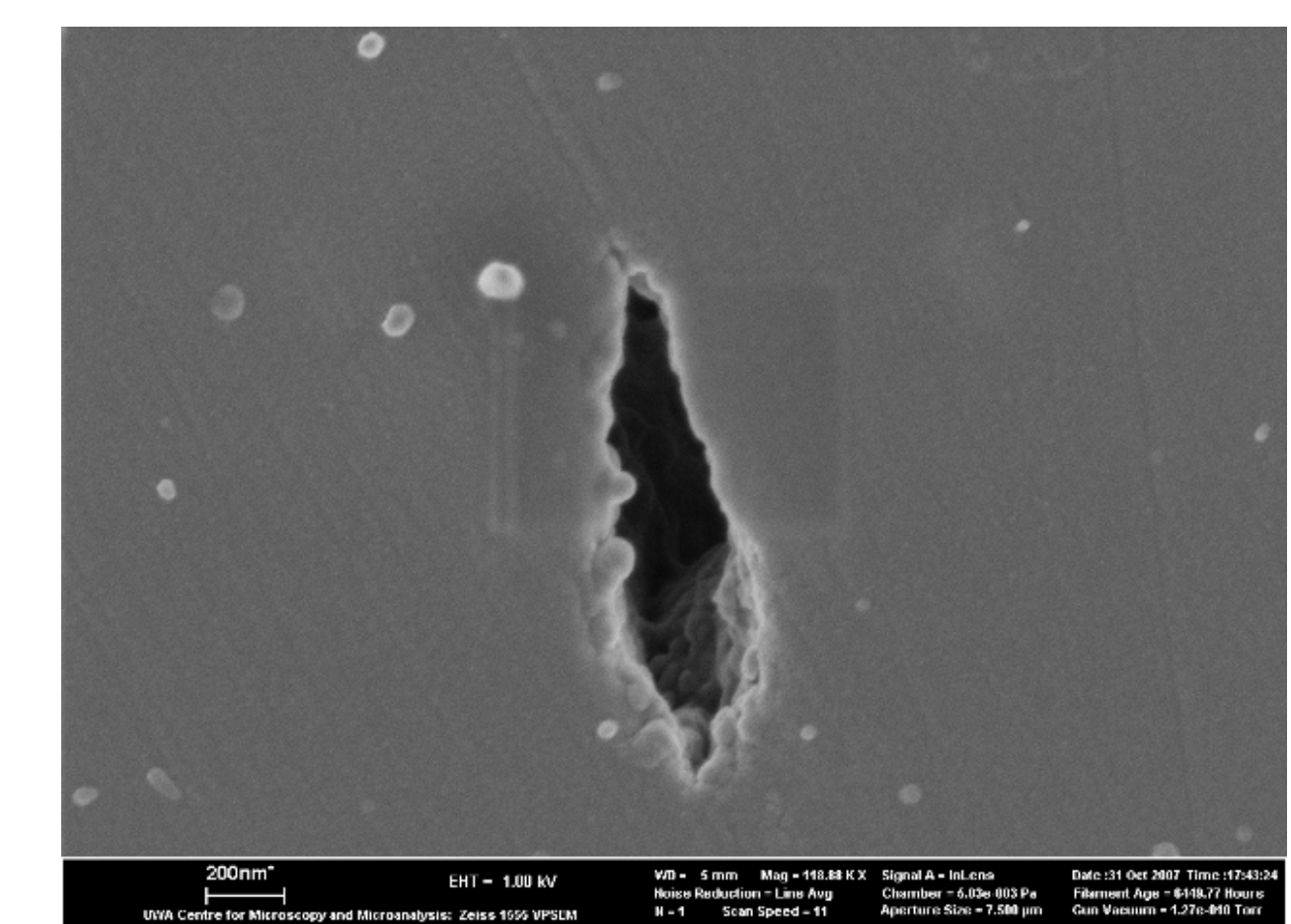
Non-Equilibrium Thermodynamics have to be considered when dissipative processes are observed. While Equilibrium Thermodynamics deals with steady states; Non-Equilibrium Thermodynamics are concerned with the transition between these steady states and the actual rate of energy dissipation (entropy production) has to be determined.

### Nano-Tomography

High energy x-ray radiation from a synchrotron is used to obtain CT images of rock samples. Resolutions down to a few hundred nanometer can be reached.

### Ductile Fracturing & Cavitation

These failure mechanisms are important at the brittle-ductile transition. Here a fracture propagates by ductile deformation at its tip. Very small syn-deformational pores (cavities) can be observed in high strain core of ductile shear zones.



### Surface Energy $\gamma = E_{COH} (Z/Z_s) N_s$

The energy associated with the creation of a new surface. It is determined by the bulk cohesive energy of the material  $E_{COH}$ , the number of broken atomic bonds per surface atom ( $Z/Z_s$ ) and the areal density of surface atoms  $N_s$ .

### Maximum Entropy Production Principle

A variational principle that describes the dissipation rate of a system that is far from equilibrium.

## Conclusion and further use of the Maximum Entropy Production Principle

Far from equilibrium thermodynamic processes lead to the formation of structures such as faulting, folding and boudinage. In classical approaches these structures are hardwired into the constitutive equations involving an arbitrary switch between rheologies. We solve the underlying energy feedback loops and show that the formation of dissipative structures can be derived directly from thermal and chemical feedback processes.

In our simulation of the thermo-mechanical coupling we have maximised the rate of dissipation as a function of shear heating. We are currently developing an extension of that formulation to chemical-mechanical coupling. This is effective at much smaller scales, but is none the less important because it will generate strain localisations visible at the outcrop and thin section scale.



## References

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