Pattern Dynamics Applied to the Kinetics of Mineral Phase Transformations

IMAF workshop 2006

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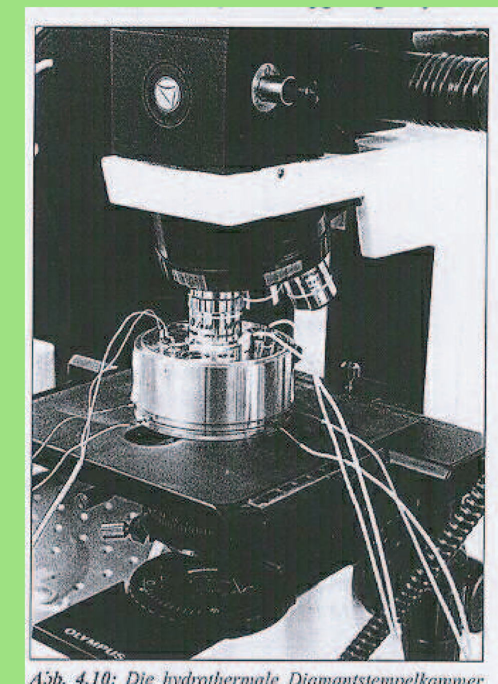
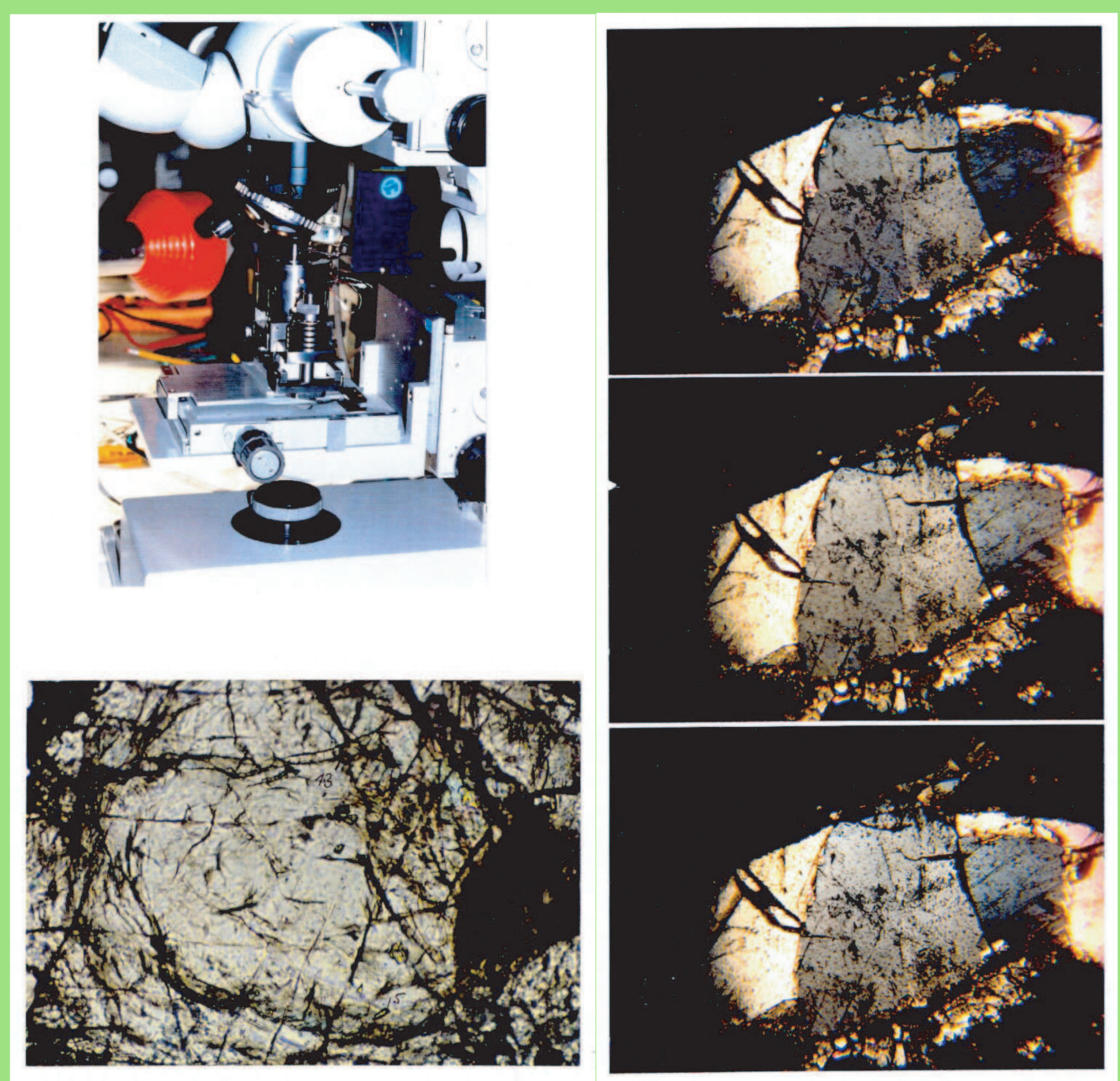
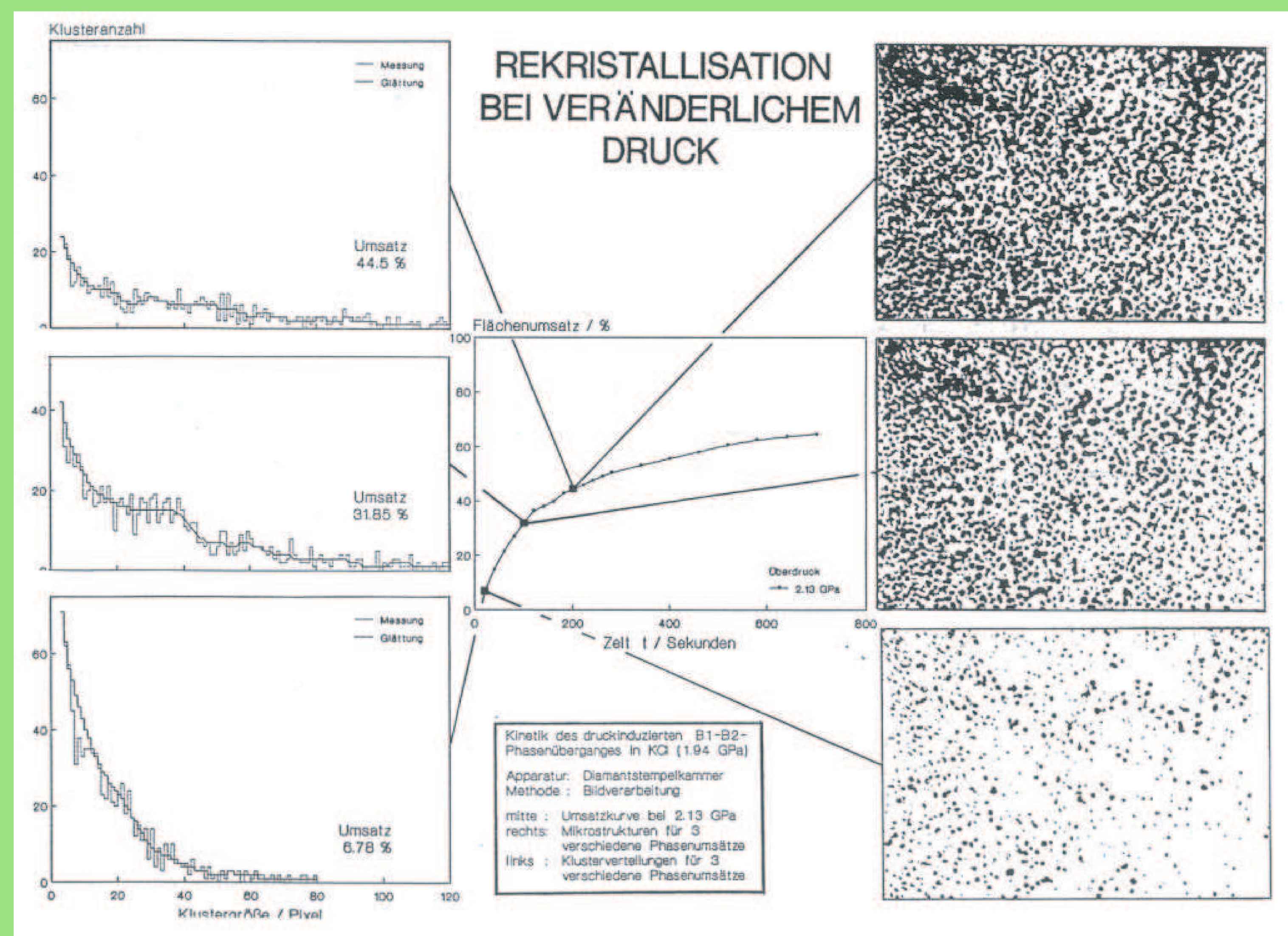


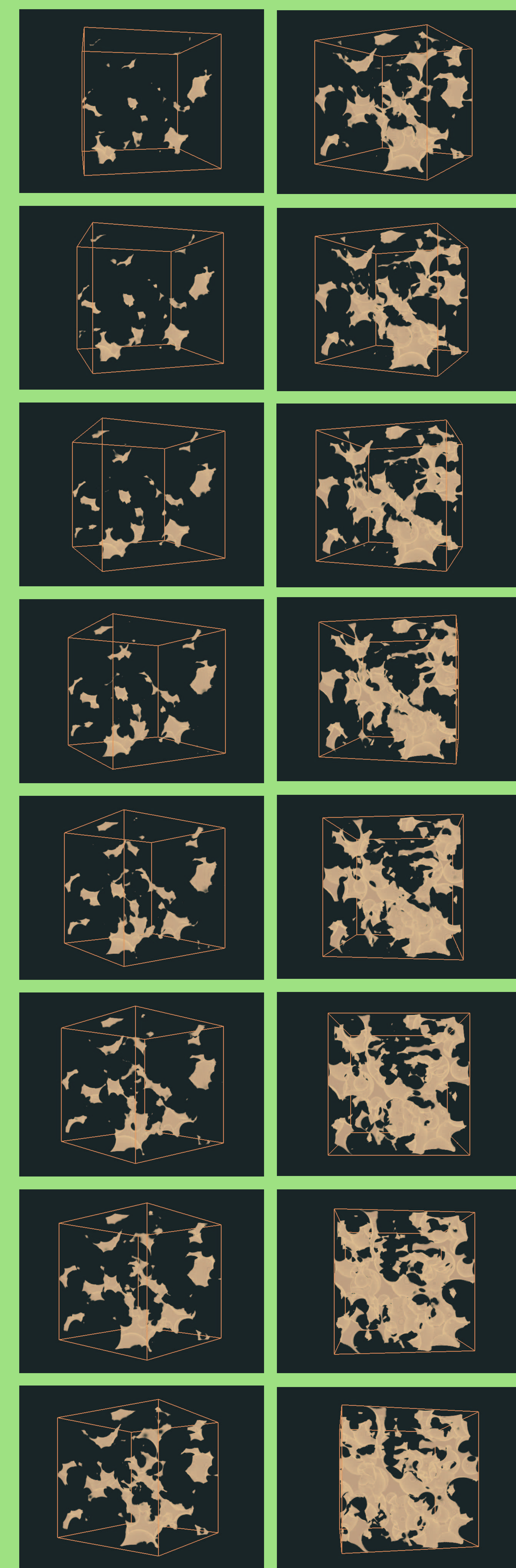
Abb. 4.10: Die hydrothermale Diamantstempelkammer (HDAC) auf dem Mikroskoptisch des Ramanspektrometers (Foto: C. Schmidt, GFZ)

(1) Experimental Setup: DAC

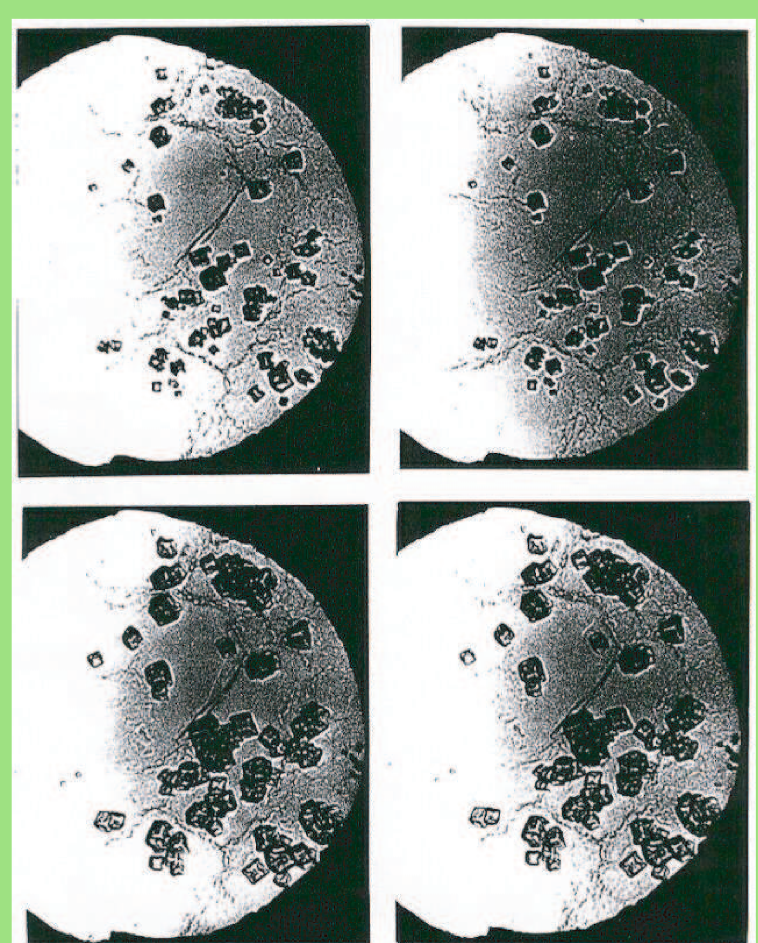


(3) time-dependent analysis of kinetic processes

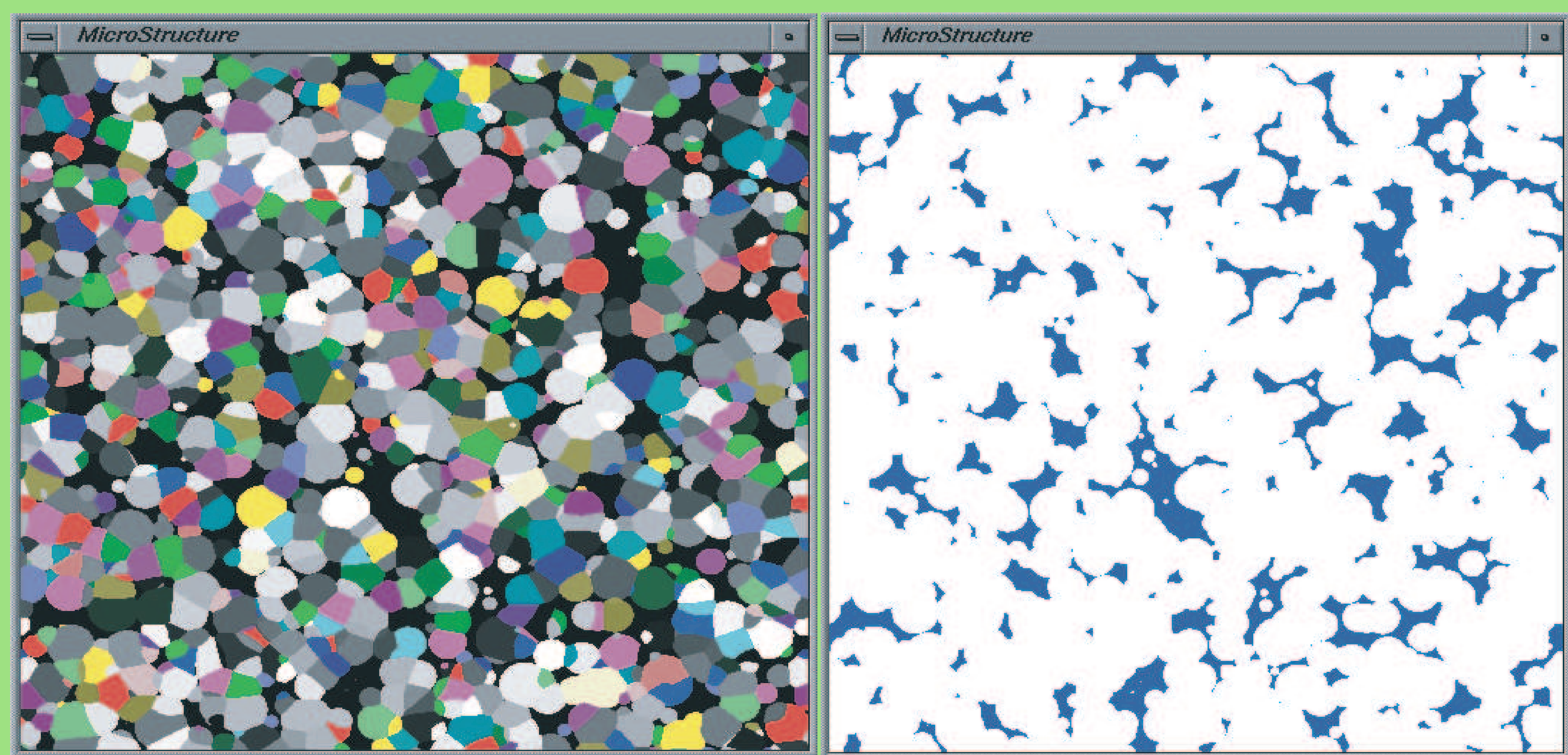




(2) snapshot images



(4) computer simulations of 3D microstructures



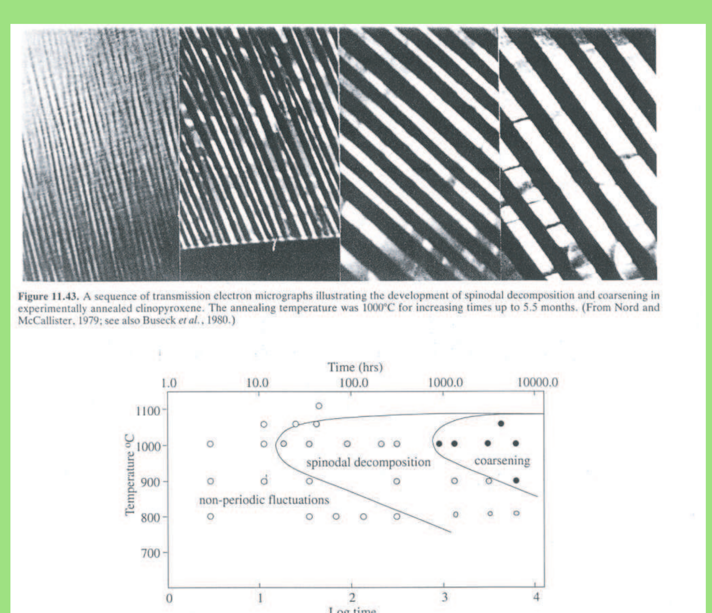
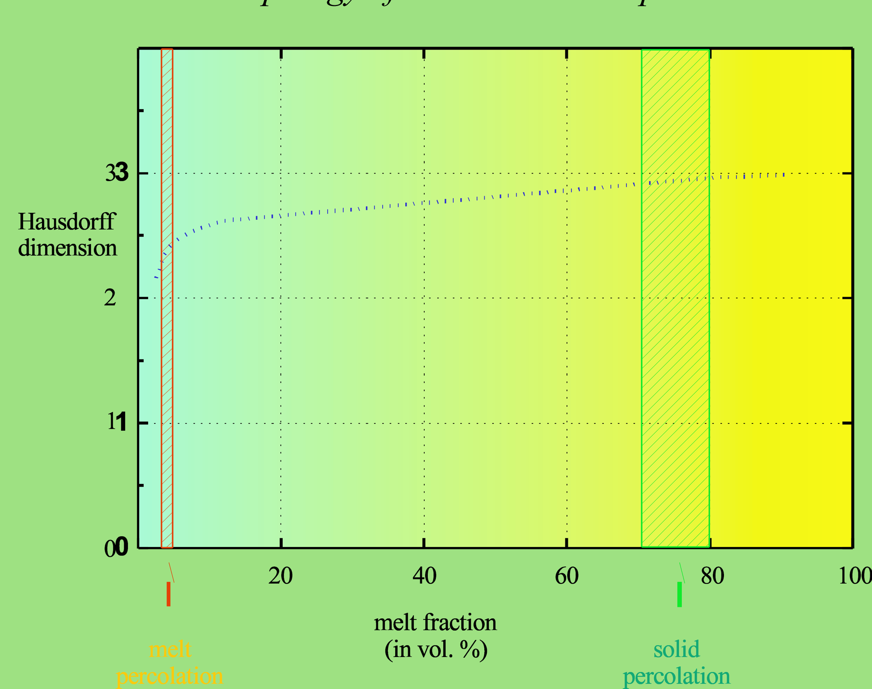


Figure 11.44. Experimentally determined TTT diagram for the spinodal decomposition of clinopyroxene of composition $Wo_{25}En_{31}Fs_{44}$ (from Nord and McCallister, 1979, see also Buseck et al., 1980).

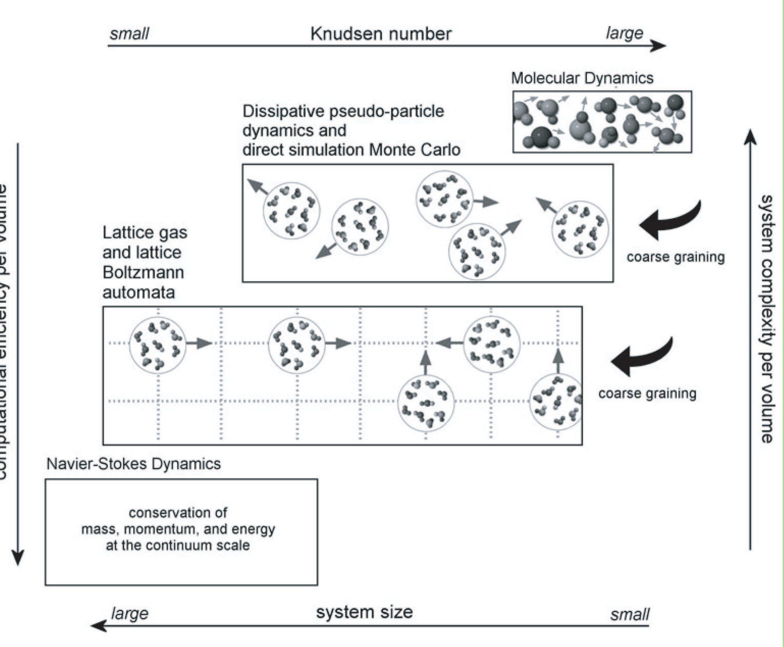
Geol. Soc. Am. Abstracts 11, 488 || In: "Pyroxenes", Rev. Mineral. 7, ed. C.T. Prewitt



(5) identification & derivation of physical transport coefficients

Overview of models in computational fluid mechanics. All approaches beyond the atomic-scale (molecular dynamics) and below the conventional continuum scale (Navier–Stokes solvers) use coarse-grained pseudo-particles which can either move on a fixed lattice (lattice-based pseudo-particle models) or continuously in space (off-lattice pseudo-particle models).

Models in computational fluid mechanics	
Molecular dynamics	
Pseudo-particle models	
Off-lattice models	Dissipative particle dynamics Direct simulation Monte Carlo methods
Lattice-based models	Lattice gas automata Lattice Boltzmann automata
Navier–Stokes solvers	



Various approaches to computational fluid dynamics together with their preferred range of applicability. Molecular dynamics methods integrate Newton's equations of motion for a set of molecules on the basis of an intermolecular potential. Dissipative particle dynamics and direct simulation Monte Carlo are off-lattice pseudo-particle methods in conjunction with Newtonian dynamics. Lattice gas and lattice Boltzmann methods treat flows in terms of coarse-grained fictive particles which reside on a mesh and conduct translation as well as collision steps entailing overall fluid-like behaviour. Navier–Stokes approaches solve continuum-based partial differential equations which account for the local conservation of mass, momentum and energy. These three methods have their respective strengths at different Knudsen numbers, where the Knudsen number is the ratio between the mean free molecule path and a characteristic length scale representing mesoscopic system heterogeneity (e.g. the obstacle size).

Permeability-Porosity Relationship

We present a model for calculating permeability of a porous solid-melt polycrystal during melting. Unlike to previous two-phase models, a solid framework is used that does not have a regular geometry nor a typical grainsize. Instead, we use a polycrystal that is created on the basis of a stochastic nucleation and growth process for first-order phase transformations as the starting state for partial melting. It is a polycrystal with continuously distributed grainsizes and random grain locations.

Permeability is then estimated through flow simulation on the constructed 3D porous two-phase body using the Lattice-Boltzmann (LB) technique. The LB method describes fluid motion with the interaction of a massive number of particles following simple local rules, rules that recover the Navier-Stokes equation at the macroscopic scale [Rothman and Zaleski, 1997].

It is known that the LB flow simulation is able to handle successfully very complex 3D pore geometries [Keehm et al., 2004]. Here, the investigated porous framework shows a fractal-like geometry near to percolation of either melt or solid phase. The flow simulation is done with an assigned pressure gradient ∇p across opposite faces of cubes. From the local flux, the volume-averaged flux $\langle q \rangle$ is then calculated using Darcy's relationship

$$\langle q \rangle = - \kappa/\eta \, \nabla p$$

where κ is the (wanted) macroscopic permeability and η is the dynamic viscosity of the melt.

References:

Keehm Y., T. Mukerji T. and A. Nur. Permeability prediction from thin sections: 3D reconstruction and Lattice-Boltzmann flow simulation. GRL, 31, L04606, doi: 10.1029/2003GL018761, 2004.

Rothman D.H. and S. Zaleski. Lattice-Gas Cellular Automata. Cambridge Univ. Press, Cambridge, 1997.

(6) Comparison with rock samples (in progress)

The formation of a basaltic melt phase along the grain boundaries of a polycrystalline rock matrix is considered as a time-reversed solidification process and is treated by a 3D computer simulation of nucleation and growth. The obtained microstructures (unconnected porosity, shape of isolated melt pockets, distribution of wetting angle, size and geometry of percolating melt cluster, permeability threshold) are analyzed and compared with experimentally obtained data for partially molten crustal protoliths (see, e.g., Laporte et al., 1997).

The resulting melt structure is in general in a good agreement with the experimental data, but becomes increasingly sensitive to the grain-scale geometry as the melt percentage decreases below 5 %, including the frequency of dry edges, the tortuosity of melt channels, and the minimum channel cross sections. It depends also significantly on a possible anisotropic growth rate of the solid-melt interphase. Because of these difficulties permeability can no longer be expressed as a simple fuction of porosity and grain-size.

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