Computer Simulation of Micromorphological Changes in Solids

Heterogeneities in solids promote stress concentrations as well as residual stresses that can influence the temporal development of the micro-morphological structure considerably. Two examples are presented in the Figure. First, PSZ-ceramics where a cubic matrix of Zirconia is, for example, stabilized by addition of MgO. Due to spatial fluctuations of the concentration of the stabilizer the cubic material may locally switch to the low temperature tetragonal crystal variant, which is different in shape and volume. Consequently, in order to accommodate this morphological change, stresses will arise in the solid that, in turn, influence the diffusion and concentration profile of the stabilizer. Eventually equilibrium is reached and rhombus-shape tetragonal precipitates result (see the left inset in the figure). Similarly, the phase separation observed tin-lead based binary solder alloys can be accelerated by combination of comparatively high temperatures and external mechanical stresses (see the second inset in the figure). It should be noted that the growth of voids observed during the last stage of loading of ductile metals is another example of such micromorphological changes. In order to describe such phenomena the local concentration field, c (or the void fraction), and the state of order, S, are typically determined from PDE's of the Cahn-Hilliard-Allen type (t denotes the time and x_i stands for the position):

$$\frac{\partial c}{\partial t} + \frac{\partial J_i}{\partial x_i} = 0 \quad ,$$

$$\frac{\partial S}{\partial t} = P_S \quad ,$$

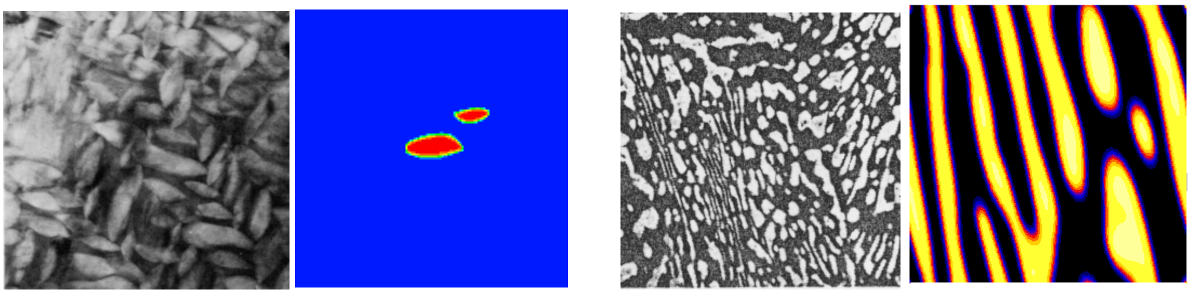
where the diffusion flux, J_i, and the production of order, P_S, are given by

$$J_i \sim -\frac{\partial}{\partial x_i}\left(\frac{\partial \psi}{\partial c} - \frac{a_{kl}\partial^2 c}{\partial x_k \partial x_l} - \frac{\partial}{\partial c}\left[\frac{1}{2}\left(\varepsilon_{ij} - \varepsilon_{ij}^*\right)\sigma_{ij}\right]\right) \quad ,$$

$$P_S \sim -\left(\frac{\partial \psi}{\partial S} - \frac{b_{kl}\partial^2 S}{\partial x_k \partial x_l} - \frac{\partial}{\partial S}\left[\frac{1}{2}\left(\varepsilon_{ij} - \varepsilon_{ij}^*\right)\sigma_{ij}\right]\right) \quad ,$$

where ψ denotes the Gibbs free energy density, ε_{ij} is the total strain, ε_{ij}^{*} is the eigenstrain (due to thermal stresses as well as to phase transitions), a_{kl} is the matrix of surface tensions, b_{kl} is the corresponding matrix for the case of the order parameter, and σ_{ij} are the Cauchy stresses.

Precise numerical data for the local stresses and strains of the complicated micro-morphologies shown in are a necessary prerequisite for the successful modeling of stress/strain coupled diffusion and order-disorder transitions (see the last two pictures in the figure). These we obtain preferably from our own micro-experiments or, if available, also from the literature.



Two examples of micro-morphological changes (experiments are juxtaposed to computer modeling) due to coupling of diffusion, change of state of order and mechanical stresses:
PSZ-ceramics, and thermo-mechanically stressed tin-lead

To model microstructural changes we use self-developed Fortran programs that involve Discrete Fourier Transforms (DFT).

In this field of research we actively collaborate with the German mathematics group of PD. Dr. W. Dreyer from the Weierstrass Institut für angewandte Analysis und Stochastik in Berlin.