Summary of thesis:

# Monte Carlo Potts Model Simulation and Statistical Mean-Field Theory of Normal Grain Growth

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Some basics of the grain structure of polycrystalline materials and especially the phenomenon of grain growth are shortly outlined (Chapter 2). In particular, the basic properties and fundamental equations are presented setting a theoretical frame for the investigation of the results of the simulation data and for the theoretical investigations.

Within the scope of this thesis the Monte Carlo Potts model method has been implemented in two and three dimensions based on the original works of Anderson et al. together with improvements in an object oriented programming language (Chapter 3). Therewith a tool has been provided to simulate complex grain structures, analyse them regarding e.g. the topology and to investigate normal grain coarsening and create therewith a basis for a statistical grain growth theory.

An initial microstructure follows after an initial period of time the well known growth law and shows the properties of self-similarity and scaling (Chapter 4).
It has been shown that the **average number of faces** $s$ and **volume change rate** $R\dot{R}$ of a given grain can be described within the quasi-stationary state by a **self-similar time-invariant function** of the relative grain size $x$. It is found that for both properties it involves a parabolic correlation. In addition, it has been shown that $s(x)$ is **not simply a binomial**, but rather a **quadratic polynomial**. This is an important point in connection with the formulation of the volume change rate in the theory. A qualitative explanation for the non-linear behaviour of $R\dot{R}(x)$ is given by relating the self-similar volume change rate directly to the number of faces of a grain representing in a statistical sense the 3D analogue to the **von Neumann-Mullins topological grain law** in 2D.

A concise and thorough formulation of statistical mean-field theories is given (Section 5.1). Following a common procedure a scaled dimensionless growth law $U$ is introduced yielding a scaled and normalised size distribution function $f(x)$, which fulfils the requirement of total-volume conservation. Originating in two different descriptions of $U$ a **generalised Lifshitz-Slyozov-Wagner (LSW) approach** and a **LSW-independent approach** is presented (Section 5.2). The generalised LSW approach is based on a growth law for Ostwald-Ripening and generalised in $U$ resulting in a **one-parameter family** of scaled and normalised grain size distribution functions showing an upper cut-off. However, in the LSW-independent approach the requirement of volume conservation can also be fulfilled if the function $U$ is rewritten using a quadratic description of $R\dot{R}$ yielding a **two-parameter family** of **scaled and normalised grain size distribution functions** that reduce for a limiting case to the above one-parameter function.

The analytical grain size distribution functions are found to **match the simulation data** (i) in direct least-squares fits, (ii) in fits using the parameters as taken from least-squares fits of the volumetric rate of change $R\dot{R}(x)$ and (iii) using a numerical integration method very well (Section 5.3).