Phase Field Modeling in Materials Science: relevant examples

Based on a phenomenological approach of phase transitions, the phase field technique consists of a “description” of any transformation by using appropriate order parameters. From a technical viewpoint, the latter can take different values, for instance 0 and 1 or -1 and +1, to distinguish between the different phases involved in the transformation; whereas they vary in a smooth and continuous manner through the interface separating two different phases. Thus, the interface should necessarily have a certain thickness allowing the continuous and smooth variation of the order parameters from one value to the other in the course of the transformation. Hence, the notion of diffuse-interface models exhibiting advantages when compared to sharp-interface models which consist of front-tracking methods. From a physical point of view, the phase transformation is studied by considering an adequate thermodynamic potential which is usually the free energy of the system and which could be the entropy in some cases. The potential is expressed as a function, of the order parameters which could be conserved such as the solute concentration or non-conserved such as the phase fields characterizing each phase. This function can be generalized to a functional comprising the gradients, of the order parameters, which denote the cost in energy related to interfaces.

The phase-field technique is largely used in materials science, to simulate microstructure’s formation, mostly in the case of alloys’ solidification and also in the case of solid-solid transformations. In the present talk, the phase field method will be presented in a fundamental and simplified manner. The application of the phase-field technique for the investigation of the discontinuous precipitation reaction will be discussed.