Computer Simulation of Microstructure Formation in Materials

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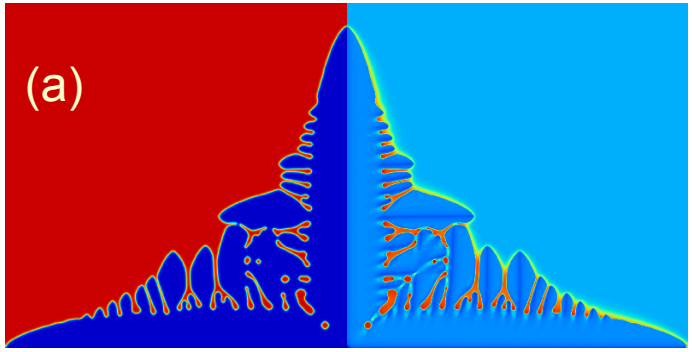
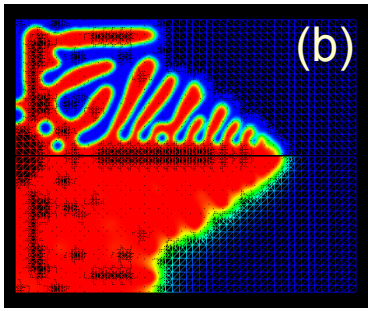
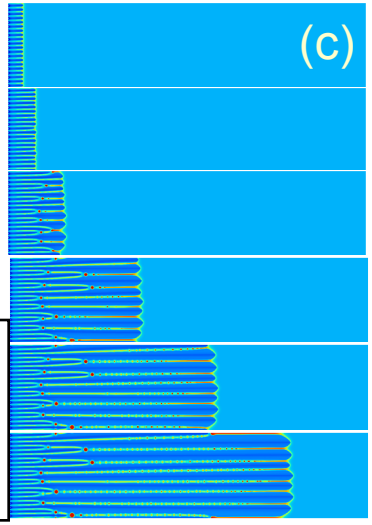
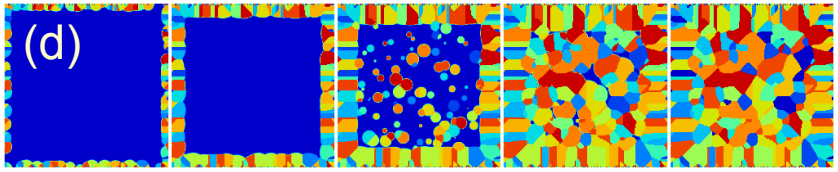






(a) Dendrite pattern
(b) FEM division
(c) Directional solidification
(d) Casting microstructure



Content:

Most engineering materials consists of complicated microstructures and it strongly affects the macroscopic material properties. Therefore, precise evaluation of the microstructure has been required. In our research group, various computational methods has been developed using molecular dynamics, phase field, and continuum mechanics. Our ultimate goal is to construct a multi-scale mechanics, and to predict the macroscopic material strength and mechanical behavior based on microscopic structure and also considering nanoscopic crystal structure and defects.

The figures in the left-hand side box are the simulation results by the phase field model. Figure (a) is a dendrite structure which is formed in a binary alloy under super-saturated condition. The left-hand half of the figure represents the phase field, and right-hand half chemical composition. Figure (b) is the finite-element mesh division for the dendritic simulation in which interfacial region has finer mesh and re-meshed as the dendrite grows. Figures (c) and (d) show the cellular structure during directional solidification, and casting structure, respectively. Such various microstructure can be simulated.

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