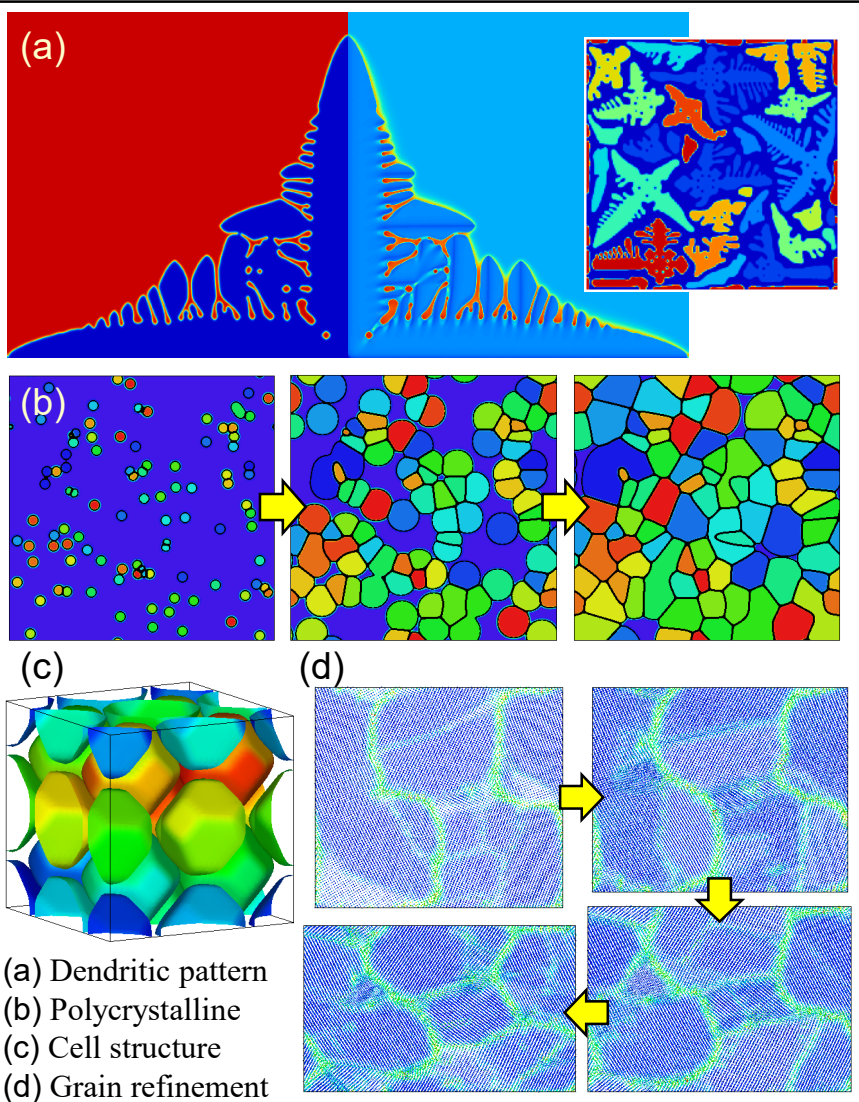


# Computer Simulation of Microstructure Formation in Materials

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## Content:

Most engineering materials consist of complicated microstructures and they strongly affect the macroscopic material properties. Therefore, precise evaluation of the microstructure is required. In our research group, various computational methods have been developed using molecular dynamics, phase-field model, and continuum mechanics. Our ultimate goal is to construct a multi-scale mechanics predicting the macroscopic material strength based on the microstructure. All the figures in the left-side box are our simulation results; (a) dendritic structure and (b) polycrystalline formation, both of which are simulated using phase-field model. Figure (c) represents a numerically modelled cell structure, which can be applied to various materials such as porous materials. Figure (d) shows grain refining process under severe compressive deformation obtained by molecular dynamics simulation. We also apply finite-element simulations to predict deformation and residual stress distribution during heat treatment such as quenching of steel.

## Appealing point:

We are trying to totally simulate complete material processing to predict deformation and strength of materials based on microscopic properties, leading to improvement of engineering products.

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