

MULTISCALE AND PHYSICAL COUPLING MODEL FOR METAMATERIALS DESIGN AND PROCESSING

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Metamaterials is a material design that embeds target functions at the material itself and seeks new performance with the object of saving of energy, or consideration of environment. There are two indispensable keywords in material design on the basis of metamaterials. They are multiscale and physical coupled modeling in consideration of mesoscopic structures.

The simulation models for material design can be classified according to the number of atoms of the target system, i.e. micro, meso and macro scales. In order to reconcile calculation efficiency and sensitivity to local information, we have to perform calculation hierarchical to space, and there is the necessity of performing a material design, which reflects the information acquired on each class mutually. This is the concept of multiscale modeling. At the same time, the phenomenon of inducing only a simple result often presents a complicated aspect by each interaction. In such a case, it is indispensable to analyze all physical phenomena simultaneously. This is the concept of physical coupling.

Surface structured material is one of the typical metamaterials. In this research, we performed the numerical simulations with use of FEM for the analysis of plasma-nitriding process that used for manufacturing surface structured materials, and we considered the applicability of multiscale and physical coupled modeling for the material design on the basis of metamaterials.

First, the numerical simulation in a 1-dimensional (1-D) system was performed for the plasma-nitriding process of Fe-Cr alloys. The governing mechanisms of the nitriding process of Fe-Cr alloys are the diffusion of nitrogen in alpha-Fe and the reaction of chromium and nitrogen. The numerical simulation was performed using the reaction-diffusion equation and we analyzed how a nitriding phenomenon changed while the change of the balance between the diffusion constant and the reaction constant in comparison with experimental results^[1].

Next, the domain to be analyzed was extended to 2-D and the numerical simulation was performed for the nitriding process of the polycrystalline aluminum in consideration of the grain boundary region. In order to analyze the nitriding process with emphasis on the influence of the total area of grain boundary region and the distribution of grain size, the homogenization method^[2] was applied to diffusion of nitrogen and we evaluated homogenized diffusion coefficient.

References

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