新学術領域「コンピューティクスによる物質デザイン：複合相関と非平衡ダイナミクス」
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# Strong ferromagnetism of quasi-one-dimensional nano-structure in Fe-Cu alloy

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Recently, spinodal decomposition is observed in Cu-Ni alloy experimentally [1] and theoretically [2]. One-dimensional nano-structure in the alloy is proposed to enhance thermoelectric properties such as Peltier effect. Moreover, we expect that this kind of structure will enhance a magnetic property of metallic alloys.

Fe is a ferromagnetic element which is cheap and common compared to Ni or Co. Therefore, the alloy of Fe and other elements is very promising to obtain a new economic magnetic material. We study the Fe-Cu alloy with 20% Fe. From phase diagram [3], Fe and Cu almost separate from each other in the mixing so that we can obtain spinodal decomposition phase in this alloy. The alloy is assumed to have FCC crystal structure. Although bulk Fe exists only at elevated temperatures (> $910^{o}$C), FCC Fe can be stabilized as particles coherently precipitated from an FCC Cu host. [4]

We simulate the Fe nano-wire surrounded by Cu matrix under a modified layer by layer crystal growth condition based upon *ab initio* electronic structure calculations by the Korringa-Kohn-Rostoker coherent potential approximation and Monte Carlo simulation of the two-dimensional spinodal nano-decomposition. Here we use MACHIKANEYAMA 2002 package developed by Akai [5].

By plotting hysteresis loops for a shape-controlled structure of the alloy in different temperatures, we propose the strong ferromagnetism of the Fe-Cu alloy enhanced by the shape anisotropy (one-dimensional structure).

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