Fabrication of CoIrMnAl Heusler alloy predicted from machine learning

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In recent years, the exploration of new materials using machine learning (ML) methods has drawn considerable attention of the researchers. Since, Heusler alloys are composed of various types of elements, and different possible combinations between the constituent elements could result enormously large number of alloys, so these alloys are attractive playground for the application of ML [1,2]. We have been developing a ML method for prediction of new compositions Heusler alloy based magnetic tunnel junctions. As a preliminary ML result, a large number of new compositions are found. Here, we focus on CoIrMn*Z* (Z=Al, Si, Ge, Ga) systems among those as a model case [Fig. 1(a)]. These alloys are predicted to show relatively high Curie temperature even though only half of constituent elements are magnetic [3]. In addition, those have lattice constants well matched to that of MgO [3], in contrary to the conventional Co_2Mn-type Heusler alloys [3]. In this study, we examined whether CoIrMnAl films can be experimentally grown. We fabricated CoIrMnAl thin films using an ultrahigh vacuum magnetron sputtering. The stacking structure was single-crystal MgO(001) substrate/ CoIrMnAl (50)/Ir (3) (thickness is nm). After the deposition of CoIrMnAl films at room temperature, *in situ* annealing was performed at various temperature T_a. We also prepared the films grown with substrate heating at different temperature T_s. We observed superlattice and fundamental diffraction peaks 002 and 004, respectively, in all samples by X-ray diffraction (XRD) [Fig. 1(b)] and confirmed single phase *B*2-ordered epitaxial films were obtained. The *B*2 order parameters were evaluated as up to 0.8. The lattice constant evaluated was very close to the theoretically predicted value, whereas the saturation magnetization and the Curie temperature were lower than the theoretical values. The difference between the theory and experiment will be discussed in terms of the site disorder. This work was in part supported by CREST (No. JPMJCR17J5).

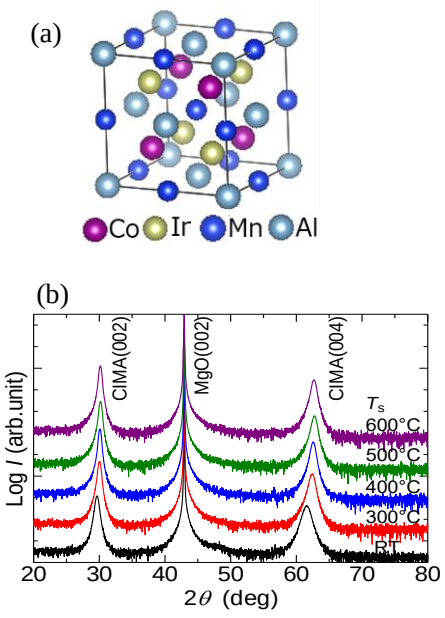

Fig. 1. (a) Crystal structure of *Y* type quaternary Heusler alloy CoIrMnAl. (b) Out-of-plane XRD patterns of CoIrMnAl films.

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