A comparison between Si substitution and pressure effects on structural and magnetic properties of tetragonal Mn₃Ge

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Mn-based materials with tetragonal structure have attracted much attention in the field of spintronics and permanent magnet [1,2], because these alloys exhibit high magnetic transition temperature and strong uniaxial magnetocrystalline anisotropy without 4f elements. Among them, Mn₃Ga and Mn₃Ge with tetragonal D₀₂₂ structure have crystallographically different two Mn sites, Mn₁ and Mn₂ sites. The magnetic moment at Mn₁ site (Wycoff position 2b site) is directed opposite to that at Mn₂ site (4d site), leading to a ferrimagnetic ordering with low magnetization of the alloys. It has been known that the magnetic properties of tetragonal Mn alloys are strongly influenced by the number of the valence electron [3,4]. On the other hand, theoretical investigations have predicted that the magnetic state corresponding to exchange interactions between the Mn sites is sensitive to structural properties such as an atomic order, an off-stoichiometry and an atomic distance [5,6]. In this study, we have investigated Si substitution and pressure effects on magnetic properties of off-stoichiometric Mn₃Ge with tetragonal D₀₂₂ structure to clarify relationship between magnetic and structural properties of the alloys.

Polycrystalline samples of Mn₃.₀₉Geₐ.₉₁-Siₓ were prepared by arc-melting method. Powder samples prepared from the ingots were aged at 673 K for a week to obtain the tetragonal D₀₂₂ phase. Structural and magnetic properties at ambient pressure were investigated by a conventional powder X-ray diffractometer and a vibrating sample magnetometer. Magnetization measurements under high pressure were performed using a superconducting quantum interference device and a piston-cylinder-type pressure cell with a liquid pressure-transmitting medium (Daphne 7373). Powder X-ray diffraction experiments at room temperature under high pressure were carried out using a diamond anvil cell with a liquid pressure-transmitting medium (Daphne 7373). From the results of high pressure X-ray diffraction experiments at room temperature, we can conclude that the D₀₂₂ structure of Mn₃.₀₉Ge₀.₉₁-Siₓ is kept up to 10 GPa. The lattice constants a and c and the unit cell volume monotonically decrease with increasing pressure. However, the axial ratio c/a is not affected by applying pressure. These results indicate that the pressure effect on the structural properties of D₀₂₂ structure is mostly same to the Si substitution effect. Magnetization of Mn₃.₀₉Ge₀.₉₁-Siₓ at ambient pressure decreases with increasing Si content. Similarly, magnetization of Mn₃.₀₉Ge₀.₉₁ decreases with increasing pressure, as shown in Fig. 1. The unit cell volume dependence of magnetization for Mn₃.₀₉Ge₀.₉₁-Siₓ is consistent with that for Mn₃.₀₉Ge₀.₉₁ under high pressure. From the results of the Si substitution and high pressure experiments, we can conclude that the Si substitution and pressure effects on magnetization are attributed to the structural properties of D₀₂₂ structure such as contraction of unit cell volume and shrinkage of atomic distance between Mn atoms.

![Figure 1. Magnetization curves at 5 K under various pressures up to 1.1 GPa for Mn₃.₀₉Ge₀.₉₁](image-url)

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