Fe_xTiS_2 層状結晶における鉄原子の秩序とその磁性の観察

Arrangement order of iron atoms and their magnetism in FexTiS2 layered structures

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Transition metal dichalcogenides can modulate their physical properties by introducing foreign species between the transition metal dichalcogenide layers. For example, when magnetic atoms are inserted into TiS_2, different magnetic behaviors have been reported depending on their concentration [1] – [2]. However, the relationship between the ordered arrangement of magnetic atoms and magnetism has never been clarified fully. One of the reasons is that the arrangement structure of magnetic atoms depending on the concentration has not been investigated in detail. In this study, Fe_xTiS_2 single crystals with Fe concentration of $x = 0.05$, 0.1, 0.15, 0.20, 0.25 and 0.33 were prepared. The purpose of this study was to clarify the ordered arrangement structure of intercalated iron atoms by systematically examining it using a spherical aberration-corrected scanning transmission electron microscope (STEM) system. In addition, these magnetization values were measured using a superconducting quantum interference device to clarify the relationship between the ordered arrangement and measured magnetism.

Annular bright field (ABF) images were observed at the thin regions to identify the arrangement of Fe atoms from the contrast difference as shown in Fig. 1 [3]. At low concentration, the Fe atoms had preferential short-range order of $\sqrt{3}a$ in the layer (a is the lattice constant). As the concentration was further increased gradually from x = 0.05, 0.10, 0.15 and 0.20, there was a tendency for the dominant order to change from $\sqrt{3}a$ to $2a$ ordering. And, x = 0.20 was found to be starting point at which 3D ordering occurred, where the $2a\times2a\times2c$ was found to be formed partically. As the concentration was further increased to 0.25 and 0.33, long-range $2a\times2a\times2c$ and $\sqrt{3}a\times\sqrt{3}a\times2c$ superstructures were identified, respectively. These experimental data suggested that at low Fe concentrations ($x \leq 0.15$), the main interactions between the Fe atoms were only intralayer interaction but at high concentrations ($x \geq 0.20$), the interlayer Fe interactions had an effect on the Fe ordering, which resulted in the 3D Fe ordering (Fig. 2). These results are in good agreement with the Monte Carlo simulations performed by another group [4].

Magnetic measurements showed that the samples displayed spin glass at $x \leq 0.15$ and ferromagnetic behaviors at $x \geq 0.20$. The switch from spin glass to ferromagnetic behavior at $x = 0.20$ matched the STEM observation at which 3D ordering of Fe atoms were observed at $x = 0.20$. This suggested that 3D ordering of Fe atoms had a large influence on the magnetic behavior displayed.

[References]
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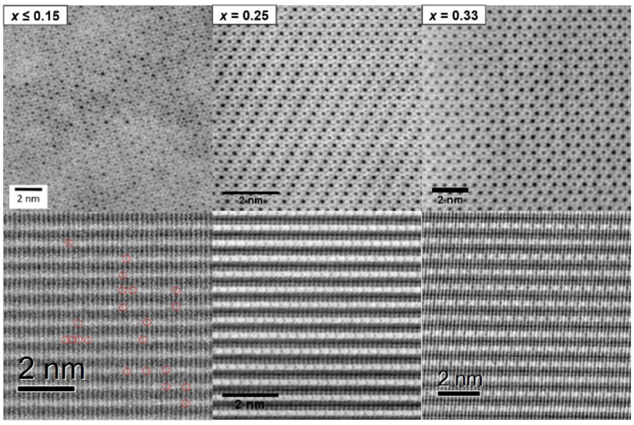

Fig. 1 ABF images of Fe_xTiS_2 layer in the [001] and [$\bar{1}$20]. The darker spots correspond to intercalated Fe atoms.