Atomic and magnetic structure in Co_xNbS_2

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The 3*d* transition-metal intercalate of the niobium dichalcogenide has a two- dimensional layered structure, in which in-plane atoms have strong ionic/covalent bondings and 3d transition metal is intercalated between the layers due to weak van der Waals forces. The crystal structure of the layered intercalate compounds gives rise to some unusual magnetic and transport properties, in that there are essentially two subsystems of electrons –those localised on the intercalate ions between the layers, and those de- localized within the host layers forming a partially filled conduction band associated primarily with the Nb d levels. Wakihara[1] has measured the temperature dependence of the electrical conductivity for the compounds Co_xNbS_2 and found that the conductivity changes from metallic into semiconducting behavior at around $x = 0.48$. They have interpreted that the dz^2 band of NbS_2 is filled with the electrons at that content by increasing Co^{2+} ions. The compound with $x = 1/3$ is antiferromagnetic[2] while ferromagnetic-like behavior with anomalies at 40 K and 90 K is observed for $x = 0.5$. In order to elucidate the origin of the strong x sensitivities in magnetic and transport properties, we have intended to study magnetic and crystal structures of compounds around $x = 0.5$ by using HERMES installed at JRR-3. Fig.1(a) shows diffraction patterns for the compound with $x = 0.51$ at 15 K and R.T. They show completely the same profiles except for some intensity changes due to the temperature effect. The result of Rietveld analysis for the 15 K data is shown in Fig1.(b). There are several unindexed peaks indicating that the sample included a few kinds of impurities. Further investigations for the compounds around $x = 0.5$ with the purified samples should be needed.

[1] M. Wakihara, *Mukizai Now* **178** (1999) 5 (in Japanese).
[2] S.S.P. Parkin, E.A. Marseglia, P.J. Brown, J. Phys. C: Solid State Phys. **16** (1983) 2765.

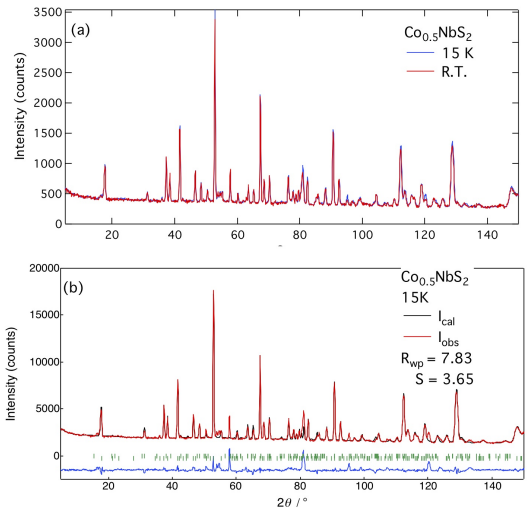

Fig. 1. (a)Diffraction patterns of $Co_{0.51}NbS_2$ at 15 K and R.T. and (b)result of Rietveld analysis for the 15 K data.