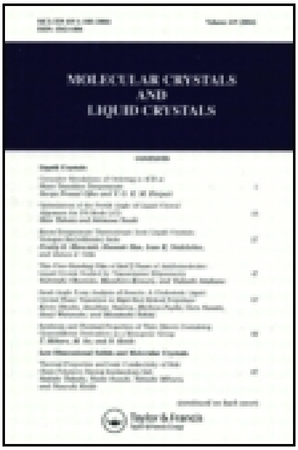

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Microscopic Studies of 2H-$NbSe_2$ Probed by Positive Muon

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Microscopic Studies of *2H*-$NbSe_2$ Probed by Positive Muon

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The microscopic state of the positively charged light particle in the transition metal dichalcogenide 2*H*-$NbSe_2$ was studied using the muon spin relaxation method (μ^+SR) and muon level crossing resonance method (μ-LCR). Muons are expected to stay at interlayer position and behaves as a hydrogen like intercalant. We discuss the relation between conduction electron properties and the muon's behavior.

Keywords: μ^+SR; Charge Density Wave; Superconductivity

INTRODUCTION

The compound *2H*-$NbSe_2$ is a *2H* type transition metal dichalcogenide. As shown in fig.1, *2H*-$NbSe_2$ possesses a layered structure with the layers weakly coupled by Van der Waals' forces. Since two dimensionality dominates the system, a weak incommensurate charge density wave (CDW) state appears below T_{CDW} ~32 K. Superconductivity (SC) coexists with the CDW state below T_{SC} ~7 K [1]. Using the muon spin relaxation method (μ^+SR) and muon level crossing resonance method (μ-LCR), we investigated the relation between the muon behavior and the CDW and SC states

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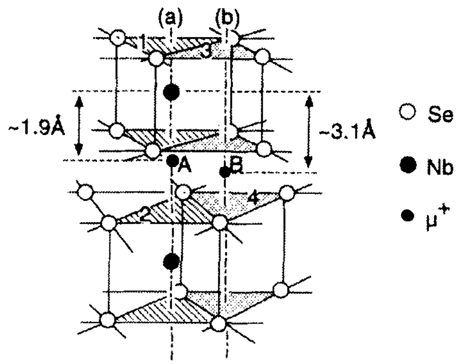

FIGURE 1: Crystal structure of *2H* type $NbSe_2$. Possible muon sites, A and B, are also shown(see text). Broken lines (a), (b) indicate the center axes of the two types of triangular prism; one type (1,2) contains Nb, while the other (3,4) does not.

in *2H*-$NbSe_2$. Transition metal dichalcogenides are known to be able to intercalate molecules or atoms into the interlayer. In *2H*-$NbSe_2$, the muon is expected to behave as a hydrogen-like intercalant and its behavior is interesting from an intercalation chemistry perspective. In addition, it is well known that the behavior of positive muons strongly depends on the conduction electron character in some cases; for example, muon quantum diffusion phenomena depend critically on the nature of the Fermi surface [2].

EXPERIMENT

Our μ^+SR and μ-LCR experiment was performed at Port 2 of the RIKEN-RAL muon facility at the Rutherford Appleton Laboratory in the UK. The standard pulsed μ^+SR method and μ-LCR method were applied. We implanted spin polarized pulsed muons parallel to the c-axis of a single crystal of *2H*-$NbSe_2$, prepared by the iodine transport method at the University of Tsukuba.

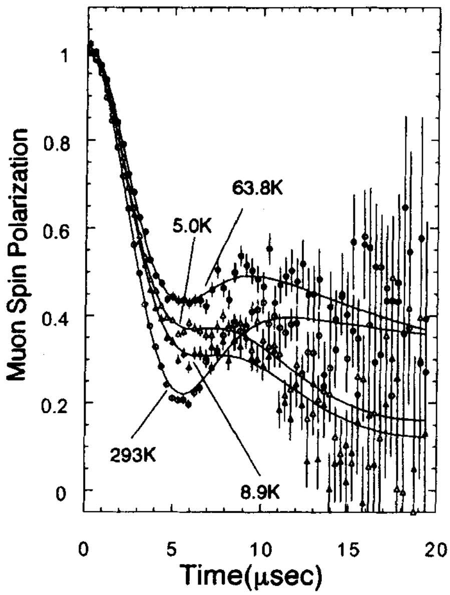

FIGURE 2: Typical ZF-μSR spectra at 293 K, 63.8 K, 8.9 K (CDW phase) and 5.0 K (CDW and SC phases).

RESULTS and DISCUSSION

Figure 2 shows typical zero field (ZF) μ^+SR spectra in *2H*-$NbSe_2$. At 293 K, Kubo-Toyabe type relaxation, which indicates that the local magnetic field at muon site is static and its distribution is Gaussian distribution [2] , was observed, probably originating mainly from the nearly static magnetic moments of the ^{93}Nb nuclei. From the ZF-μ^+SR data at low temperatures and the transverse field μ^+SR data in the field-cooled SC phase, under the field cooling procedure, we confirm that the spins of about 20% of the implanted muons into the sample were depolarized much more slowly than those of the remainder at 293 K. Interestingly, the ratio between the Kubo-Toyabe component ("fast component") and the slowly depolarizing component ("slow component") was temperature-dependent. As shown in fig.3, the asymmetry A_1 undergoes a sudden decrease with decreasing temperature at T_X=140 K. No phase transition is known at 140 K, but it may

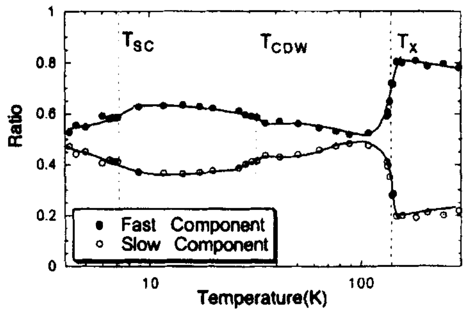

FIGURE 3: Temperature dependence of the ratio of fast and slow component.

be that our data shows a new phase transition. Alternatively, it might be possible to interpret the results in terms of trapping/detrapping of muons at vacancies or impurities in the crystal as was observed in Nb [4], where the trapping potential corresponded to ~140K.

A significant change of the muon states is also observed at T_{CDW}. Below T_{CDW}, the amplitude of the fast component slightly increases with decreasing temperature. In addition, there is a clear increase of the muon spin relaxation rate in the time region $t > 10$ μsec. These facts clearly show that the muon states are affected by the CDW state. At T_{CDW}, an energy gap appears in the Fermi surface and the density of states (DOS) decreases. It is known that hopping motions of muons in a metal are related to the conduction electrons near the Fermi surface through the electron-drag effect, with the hopping rate increasing in the SC phase [2]. Although the muons of the slow component might be diffusing above T_{CDW}, the muon spins of the slow component begin to be depolarized below T_{CDW}, which is not consistent with the electron-drag effect. Below T_{SC}, the fast component decreases with decreasing temperature as shown in fig. 3, and the muon spin relaxation rate is slightly slower than that above T_{SC}. Below T_{SC}, the DOS at the Fermi surface disappears due to the BCS gap, and the behavior of the slow component might therefore be related to the influence of the BCS gap.

The experimentally-obtained dipolar widths at the muon sites are $\Delta_1/\gamma_\mu \sim 3.9$ G for the fast component and $\Delta_2/\gamma_\mu \sim 1.1$ G for the slow

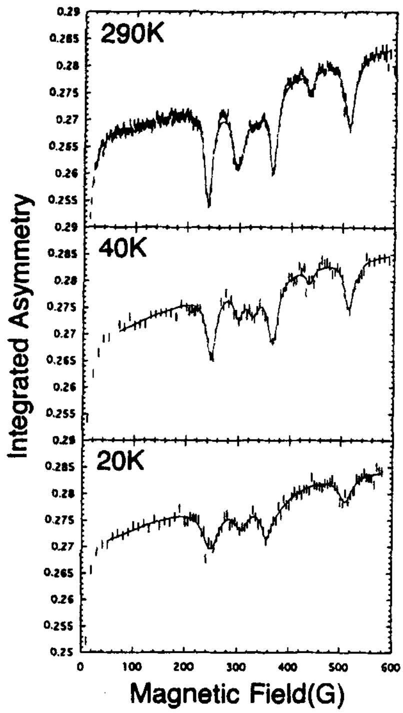

FIGURE 4: Longitudinal magnetic field dependence of the integrated asymmetry.

component. Assuming that the muons are located at the centers of the triangular prisms, the dipolar fields of the ^{93}Nb nuclei are estimated to be ~3.9 G and 1.3 G at site (A) and site (B) in fig. 1, respectively. Thus we suppose the muons to exist at the interlayer position, taking the role of intercalant.

To know the detail of the local states of *2H*-$NbSe_2$ and muon state, we have applied level crossing resonance (LCR) method. ^{93}Nb nuclei has spin $J=\frac{9}{2}$ and quadrupole moment $Q=0.16\times 10^{-24}\text{cm}^2$. The muon level crossing resonance occurs when quadrupolar splitting energy at ^{93}Nb site matches with a corresponding Zeeman splitting energy of muon in a magnetic field and muon spin is depolarized at a matching field. Figure 4 shows the dependence of applied longitudinal field on the integrated asymmetry, which defined as $(N_F - N_B)/(N_F + N_B)$, which corresponds to the muon spin polarization. Here, N_F and N_B are the total number of emitted positrons counted at forward counters and backward counters, respectively. As shown in Fig.4, we can clearly see the six resonance peaks. We found that the amplitudes of LCR peaks are reduced below 30 K. This feature clearly shows the effects of the CDW state. We have not observed significant change of the μ-LCR spectra at 140 K, which indicate that there is unlikely to be a large modification of the crystal structure at 140 K. To know the details of the muon position and of the local state of *2H*-$NbSe_2$, theoretical calculation is required.

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