

Response of Magnetic Field by Conduction Electrons at Low Temperature in 2H-NbSe₂

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Abstract

Here, we have presented the magneto-resistance (MR) on polycrystalline and single crystal of 2H-NbSe₂. The obtained MR on single crystal shows anisotropic nature associated with small longitudinal MR i.e. $(\Delta\rho/\rho_0)_{\parallel}$ in which $H \parallel$ direction of current flow compared to transverse MR i.e. $(\Delta\rho/\rho_0)_{\perp}$ in which $H \perp$ direction of current flow. This anisotropy behaviour is associated with the complex Fermi surface found from the analysis of two-band model and Kohler's rule.

Keywords: Transition metal compound, magneto-resistance, two-band model, Kohler's rule

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INTRODUCTION

The chemical composition of transition metal dichalcogenide compounds (TMDC) is represented by MX₂, where M= transition metal atom and X=S, Se and Te, in which M-atoms are sandwiched between two X-layers. 2H-NbSe₂ is one of TMDC, which shows trigonal prismatic coordination. Its high purity compounds show a charge density wave (CDW) at 35 K followed by a superconducting (SC) transition at 7.3 K [1–7]. Due to the coexistence of these two transitions in 2H-NbSe₂, the scientific community has been contributed lots of information by different ways [8–18]. Regardless of its SC transition, the CDW transition is found very sensitive to residual resistance ratio (RRR), which measures the purity of the compounds [2].

Here, we have presented the magneto-resistance (MR) data of 2H-NbSe₂ in both single crystal and polycrystalline compounds of 2H-NbSe₂. This MR provides the hypothetical picture of the Fermi surface, which depends on the concentration of electrons.

EXPERIMENTS

The polycrystalline compound of 2H-NbSe₂ is prepared by solid-state reaction method from high purity elements in an evacuated sealed quartz tube at 700°C. Then single crystals are

grown by chemical vapour transport technique at 750°C from the above polycrystalline compounds, same as reported earlier [1]. The single phase of hexagonal structure with lattice constants $a \approx 3.445 \text{ \AA}$ and $c \approx 12.551 \text{ \AA}$ are calculated from room temperature X-ray diffraction on polycrystalline compounds. Then magneto-resistance (MR) is measured below 10 K by applying magnetic field parallel and perpendicular to the single crystal plane of NbSe₂ along which current is passed. The lowering of compound temperature is achieved through a cryogenic free Helium close cycle refrigerator.

RESULTS AND DISCUSSION

Magneto-Resistance

The temperature dependence resistance with and without field on 2H-NbSe₂ polycrystalline and single crystal are reported elsewhere [19]. From that, one can easily notice the existence of positive MR. In single crystal, the longitudinal MR is found small compared to transverse MR. But in polycrystalline compound, however, the MR is very close to the longitudinal MR of single crystal. This anisotropy can be understood from two-band model and Kohler's rule as discussed below. The two-band model is based on the concentrations of charge carriers in the two bands which can at present be used to discuss the anisotropic and saturation effects of MR in

large fields. The two-band model [20] for metal is given by:

$$\frac{\Delta\rho}{\rho_0} = \frac{(H/ec)^2 \left(\frac{\sigma_{01} + \sigma_{02}}{n_1 + n_2} \right)^2 \frac{\sigma_{01}\sigma_{02}}{(\sigma_{01} + \sigma_{02})^2}}{1 + (H/ec)^2 \left(\frac{n_1 - n_2}{n_1 n_2} \right)^2 \left(\frac{\sigma_{01}\sigma_{02}}{\sigma_{01} + \sigma_{02}} \right)^2} \quad (1)$$

Here, we have assumed two types of charge carriers having n_1 electron concentration and n_2 hole concentration which gives rise to σ_{01} and σ_{02} conductivity respectively. If external magnetic field ' H ' is small then $\Delta\rho/\rho_0 \sim H^2$; but for high fields, it has two solutions at $n_1 = n_2$ provides anisotropic effect and $n_1 \neq n_2$ provides saturation effect. But Kohler's rule is used to discuss about the motion of charge carriers associated with a universal mean free path or scattering time.

Two-Band Model

For the anisotropic behaviour of $\Delta\rho/\rho_0$ in 2H-NbSe₂, we assumed the case of equal density of states in both bands i.e. $n_1 = n_2 = n$ which implies that; $\sigma_{01} = \sigma_{02} = \sigma_0/2$.

Then $\Delta\rho/\rho_0$ in SI unit is represented as follows:

$$\frac{\Delta\rho}{\rho_0} = \frac{\sigma_0^2}{(2ne)^2} H^2 = \left(\frac{e\tau}{2m} \right)^2 H^2 \quad (2)$$

This expression is equivalent to a straight-line equation with zero intercept constant, which provides information about the scattering time (τ) of the charge carriers. The fractional change in MR ($\Delta\rho/\rho_0$) around 8 K is plotted with respect to H^2 for 2H-NbSe₂ single crystal and polycrystalline in Figure 1, which clearly shows that the MR rapidly increased in $(\Delta\rho/\rho_0)_\perp$ i.e. $H \perp$ plane of NbSe₂ compared to $(\Delta\rho/\rho_0)_\parallel$ i.e. $H \parallel$ plane of NbSe₂. From the slope of $\Delta\rho/\rho_0$ vs. H^2 , however, we have calculated average scattering time $\sim 1.48 \times 10^{-12}$ sec in $(\Delta\rho/\rho_0)_\perp$ for single crystals. This scattering time is found to be reduced $\sim 5.11 \times 10^{-13}$ sec and 2.53×10^{-13} sec in $(\Delta\rho/\rho_0)_\parallel$ below and above 3 Tesla in 2H-NbSe₂ single crystal respectively. But in case of polycrystalline compound, it is found $\sim 4.55 \times 10^{-13}$ sec very close to $(\Delta\rho/\rho_0)_\parallel$ scattering time.

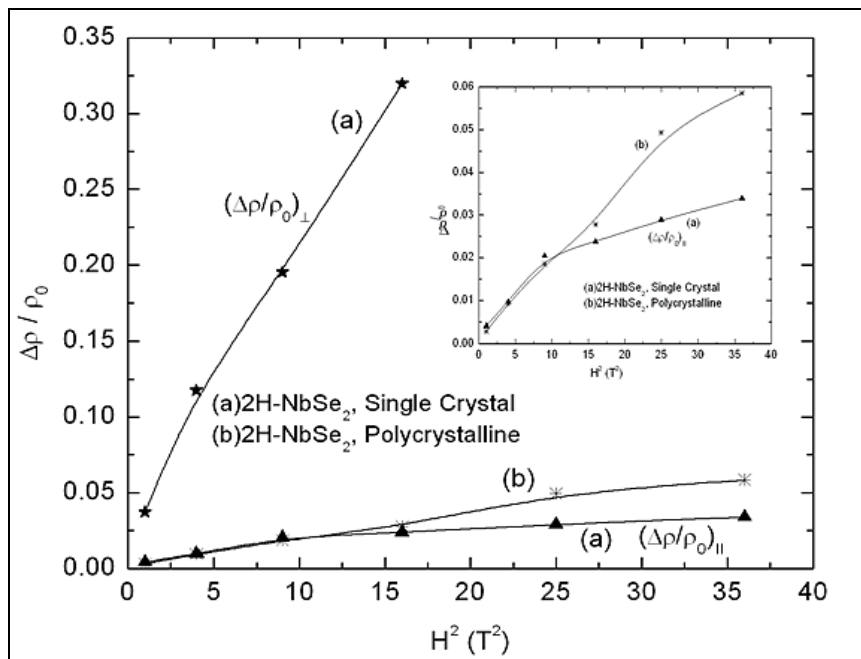


Fig. 1: $\Delta\rho/\rho_0$ vs. H^2 for 2H-NbSe₂ Single Crystal and Polycrystalline Compounds.

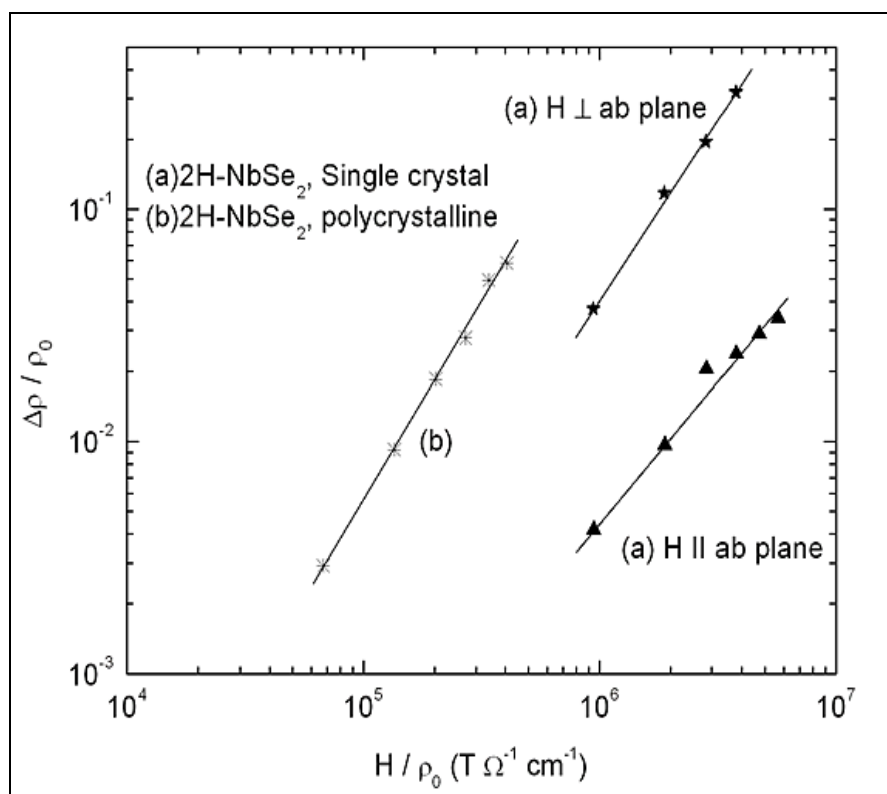


Fig. 2: $\Delta\rho/\rho_0$ vs. H/ρ_0 for 2H-NbSe₂ Single Crystal and Polycrystalline Compounds.

Kohler's Rule

Although this rule is derived only for the isotropic model of closed Fermi surface, it describes experimental data better than $\Delta\rho/\rho_0 \sim (\Omega\tau)^2$ where $\Omega = eH/2m$ in SI unit and $\tau =$ scattering time. Then non-linear behaviour of $\Delta\rho/\rho_0$ in metallic compounds are described by Kohler's rule as given below [20]:

$$\frac{\Delta\rho}{\rho_0} = f\left(\frac{H}{\rho_0}\right) \sim \left(\frac{H}{\rho_0}\right)^p \quad (3)$$

Eq. (3) implies that $\Delta\rho/\rho_0$ is a function of H/ρ_0 . Suppose, if p is the exponent of H/ρ_0 then depending on the value of p , metals are divided in to two groups: group-1 if $2 \geq p \geq 1$ and group-2 if $p < 1$. In group-1, the MR rises to infinity with H/ρ_0 whereas in group-2 MR saturates at finite value of H/ρ_0 .

On the other hand, the movement of charge particle in a constant energy surface between

the zones known as open orbit provides the increase of MR to infinity and saturation of MR at finite value of H/ρ_0 is related to the movement of charge particle within the single zone known as closed orbit.

In Figure 2, the fractional change in MR ($\Delta\rho/\rho_0$) around 8 K is plotted with respect to H/ρ_0 for 2H-NbSe₂ single crystal and polycrystalline in log-log scale known as Kohler's plot. Within the applied magnetic field of 6.0 Tesla, the exponent is found ~ 1.6 in $(\Delta\rho/\rho_0)_\perp$ and ~ 1.2 in $(\Delta\rho/\rho_0)_\parallel$. As both the exponents are greater than one, at present, we can say that there exist multiple connected Fermi surfaces along which the charge particles move. But the difference in exponent implies the anisotropy scattering same as we found in two-band model. Though $(\Delta\rho/\rho_0)_\perp$ of polycrystalline compound is very close to single crystal, it can't be compared with single crystal because the MR obtained in polycrystalline compound is an effect of average over the separate crystallites.

CONCLUSION

Here, we have tried to figure out a hypothetical Fermi surface in 2H-NbSe₂ using low temperature MR data. Regardless of 2H-NbSe₂ polycrystalline $\Delta\rho/\rho_0$, the single crystal shows anisotropic nature of $\Delta\rho/\rho_0$. First we have attempted to describe this anisotropy by two-band model with the condition $n_1 = n_2$. But it fails to account the reason for saturation like behaviour above 3Tesla with small magnitude in $(\Delta\rho/\rho_0)_{II}$ as shown in Figure 1. Therefore, Kohler's plot as shown in Figure 2 is used to understand it through electron path in k -space which follows lines of constant energy perpendicular to the direction of magnetic field. As a consequence, a complex Fermi surface is established associated with different scattering time along different direction.

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