Critical field of 2H-NbSe$_2$ down to 50mK

Adel Nader$^1$ and Pierre Monceau$^2$

Abstract

Critical field of 2H-NbSe$_2$ is determined for the field perpendicular to the conducting planes down to 50 mK, by magnetoresistance measurements. It is the first time that such a measurement is extended below 1 K. Variations are almost linear down to 1 K, with a little upward curvature, and the slope of $H_c^\perp(T)$ decreases below 1 K. The reduced critical field extrapolates to 0.9 when the temperature approaches zero, higher than the WHH upper limit of 0.69 conformably with the extension of this model for anisotropic superconductors.

Angular dependence of the critical field is also determined at 5.5 K. Variations are the same as expected for a 3D-anisotropic superconductor and the anisotropy value confirms previous results.

Keywords: Critical fields; 2H-NbSe$_2$; Layered superconductor

Introduction

The structure of 2H-NbSe$_2$ consists of three-layer packets, inside which the layers are ordered in the Se-Nb-Se sequence with covalent binding between them, whereas the packets are bound by van der Waals coupling. Due to this weak coupling in the dichalcogenides family, adjacent packets may be oriented in different ways relative one to another and as a consequence the possibility of polytypism. The most widely encountered polytype for NbSe$_2$ is the 2H, where 2 is the number of packets in the unit cell and H stands for hexagonal. The structure of 2H-NbSe$_2$ was reviewed by Meerschaut and Deudon (2001).

This compound has been extensively studied for its superconductivity and the formation of a CDW state. It shows a superconducting transition at 7.2 K (Toyota et al. 1976, Sanchez et al. 1995, Soto et al. 2007) with an upper critical magnetic field anisotropy, induced by the layered structure, of about 3.

The CDW state appears in 2H-NbSe$_2$ below $T_{CDW} \sim 33$ K (Moncton et al. 1977, Higemoto et al. 2003). It can be seen as an anomaly in the resistivity curve that the amplitude is tightly proportional with the sample purity (Iwaya et al. 2003).

An interesting aspect in the superconducting state of this compound which still attracts lots of attention is the peak effect (Banerjee et al. 1998). This effect appears as a maximum in the critical current curve in function of temperature.

Another interesting aspect in this compound is the two gaps structure (Huang et al. 2007, Rodrigo and Vieira 2004) which was evidenced, mainly, by specific heat measurement under magnetic field.

Though, it has been believed for a long time that 2H-NbSe$_2$ has just an anisotropic superconducting gap and some experimental results were explained into this framework (Toyota et al. 1976)

The behavior of the critical magnetic field has been subject to discussion since the seventies since its behavior depends tightly on the Fermi Surface geometry. As a result many theoretical calculations (Werthamer et al. 1966, Arai and Kita 2004) concluded that the critical field perpendicular to the layers vary linearly near $T_c$ and its slope decreases at lower temperatures. Though an upward curvature is expected for the critical field in the parallel direction (Arai and Kita 2004).

The perpendicular critical field saturation at very low temperatures has never been investigated experimentally.

In this work critical magnetic field of this compound is determined by mean of magneto-resistance measurement down to 50mK for the first time. It shows a behavior as expected by theoretical models mentioned above with almost a linear variations near $T_c$ and a slope decreases at very low temperature. Angular dependence of the critical field is also determined at 5.5 K, it confirms previous results.
Experimental details

The NbSe$_2$ powder is prepared starting from constituting elements at stoichiometric ratio, and then the crystals are grown by thermal gradient using the iodine as a transport agent. Single crystals of these compounds are in platelet form with a diameter in the range of 2 mm and a thickness of 50 $\mu$m.

Measurements down to 50 mK are done using a top loading dilution refrigerator and a 8 Tesla superconducting magnet. The anisotropy is measured at 5.5 K using a rotating system with an accuracy of 0.1°.

Results and discussion

Our best sample, of the sharpest transition has a critical temperature at half height of normal state resistance of 7.0 K, with a transition width of about 0.8 K, as shown in Figure 1.

The upper critical magnetic field is taken at half height of the measured magneto-resistance. Figure 2 shows variations of $H_{c2} (T)$. It shows a little upward curvature near $T_c$. Though, by experience, upward curvature near $T_c$ may be induced by a rather wide resistive transition, a better discussion of such an aspect would then need a better quality sample, with a sharpest transition. Nevertheless, such an upward curvature was expected by Arai and Kita (2004) for the parallel critical field or for layer compounds of higher anisotropies (Woollam et al. 1974).

Below 1 K the slope of $H_{c2} (T)$ decreases as expected by Werthamer et al. (1966) for a dirty superconductor and by Arai and Kita (2004)).

Our results are similar to that found in (Toyota et al. 1976) where the measurements were done only down to 1.3 K. Though, no upward curvature near $T_c$ was mentioned in (Toyota et al. 1976), probably because samples were of a much better quality; their RRR ratio was always higher than 30, although, for our sample it is less than 10.

Figure 3 shows $h (t)$, which is the upper critical field normalized as in (Werthamer et al. 1966) i.e. $t = T / T_c$, and

$$h = H_{c2} / (dH_{c2}/dt) .$$

$h (t)$ extrapolates to 0.9 when $t \rightarrow 0$.

Werthamer et al. (1966) extended the calculation of the upper critical field for a bulk superconductor by taking in account Pauli spin paramagnetism and spin-orbit impurity scattering. According to this model this value should not be greater than 0.69. Though, in (Hohenberg and Werthamer 1967) it was shown that this is possible for anisotropic superconductors when Fermi surface is no more spherical.

Also, the sketch of $h (t)$ seems to be in good agreement with the reduced critical field curve calculated using the Fermi surface obtained by local density approximation (LDA) by Arai and Kita (2004) (see Figure 1 in this reference). According to this calculation $h (0)$ extrapolates to about 0.95.

Figure 4 shows variations of $H_{c2} (\theta)$ at 5.5 K, where $\theta$ is the angle between the conducting planes and the magnetic field. The following formula was given by Lawrence and Doniach (1971):

$$H_{c2} (\theta, T) = eH_{c2} (T) (\epsilon^2 \sin^2 \theta + \cos^2 \theta)^{1/2}$$

\[(1)\]
Figure 2 Critical magnetic field down to 50 mK. Continuous line is a guide for eye. Note the saturation below 1 K.

Figure 3 Critical magnetic field in reduced coordinates. Continuous line is a guide for eye. Note the value of \( h(0) \).
where $\epsilon$ is the ratio of the parallel critical field to the perpendicular one at $T$.

The fit with this formula gives an anisotropy of 3.2. This value approaches those found in (Toyota et al. 1976, Sanchez et al. 1995).

Though, Lawrence and Doniach simple model based on the effective mass anisotropy was proven not to be sufficient to describe the critical field anisotropy in layered superconductors as shown by Toyota et al. (1976) and that other assumptions should be made such as the gap anisotropy, but it could be used as a first approximation to extract anisotropy from the $H_{c2}(\theta, T)$ curve.

Let us note also that the critical field anisotropy is temperature dependent, and the parallel critical field shows an upward curvature in (Toyota et al. 1976, Muto et al. 1973).

In plane and out-of-plane coherence lengths are then $\xi_{||}(0) = 74$ Å and $\xi_{\perp}(0) = 23$ Å respectively. $\xi_{\perp}(0)$ is much greater than the distance separating the centers of two successive conducting planes, which confirms that $2H$-NbSe$_2$ is a 3D-anisotropic superconductor.

Coherence lengths as well as the critical field anisotropy are of the same range as found in (Sanchez et al. 1995) by specific heat measurements.

**Conclusion**

Critical magnetic field measurement of $2H$-NbSe$_2$ is extended down to 50 mK. The slope of $H_{c2}(T)$ decreases below 1 K and varies almost linearly near $T_c$ with a little upward curvature, probably induced by a rather large superconducting transition.

Also, the anisotropy is the same as obtained in previous works.

**Competing interest**
The authors declare that they have no competing interests.

**Authors’ contribution**
This work is a part of the PhD work of A.N where P.M was his advisor. Both authors read and approved the final manuscript.

**Acknowledgement**
I wish to thank Prof. I. Othmann Director General of Atomic Energy Commission of Syria for his support.

**Author details**
1 Atomic Energy Commission of Syria, Department of Physics, P.O Box 6091, Damascus, Syria. 2 Institut Néel CNRS/UJF UPR2940, 25 rue des Martyrs BP 166, Grenoble, Cedex 38042, France.

**Received:** 14 June 2013 **Accepted:** 26 December 2013 **Published:** 9 January 2014

**References**
Arai M, Kita T (2004) Ab initio calculations of $H_{c2}$ for Nb, NbSe$_2$, and MgB$_2$. J Phys Soc Jpn 73:2924–2927
Banerjee SS et al (1998) Generic phase diagram for vortex matter via a study of peak effect phenomenon in crystals of $2H$-NbSe$_2$. Physica C 308:25–32
Higemoto W, Nagamine K, Kuroda S, Takita K (2003) Charge density wave in $2H$-NbSe$_2$ probed by muons. Physica B 326:540–544
Hohenberg PC, Werthamer NR (1967) Anisotropy and temperature dependence of the upper critical field of type-II superconductors. Phys Rev 153:493–497
Huang CL et al (2007) Experimental evidence for a two gap structure of superconducting NbSe$_2$: a specific-heat study in external magnetic fields. Phys Rev B 76:21250
Iwaya K et al (2003) Electronic state of NbSe$_2$ investigated by STM/STS. Physica B 329-333:1598–1599
Lawrence WE, Doniach S (1971) Theory of layer structure superconductors. Proc. 12th int. Conf. on Low Temp. Phys., ed. E. Kanada (academic 1971), pp 361–362

![Figure 4](image-url)  
**Figure 4** Critical magnetic field in function of the angle between conducting planes and magnetic field at 5.5 K. Continuous line is the fit with Lawrence and Doniach expression. The anisotropy is 3.2
Meerschaut A, Deudon C (2001) Crystal structure studies of the 3R-Nb1.09S2 and the 2H-NbSe2 compounds: correlation between nonstoichiometry and stacking type (= polytypism). Mater Res Bull 36:1721–1727

Moncton DE, Axe JD, Di Salvo FJ (1977) Neutron scattering study of the charge-density wave transitions in 2H-TaSe2 and 2H-NbSe2. Phys Rev B 16:801–819

Muto Y et al (1973) Temperature dependence of ratio, $H_{c2}/H_{c2\perp}$, for NbSe2. Phys Lett 45:99–100

Rodrigo JG, Vieira S (2004) STM study of multiband superconductivity in NbSe2 using a superconducting tip. Physica C 404:306–310

Sanchez D, Junod A, Muller J, Berger H, Levy F (1995) Specific heat of 2H-NbSe2 in high magnetic fields. Phys B 204:167–175

Soto F et al (2007) Electric and magnetic characterization of NbSe2 single crystals: Anisotropic superconducting fluctuations above T. Physica C 460-462:789–790

Toyota N et al (1976) Temperature and angular dependences of upper critical fields for the layer structure superconductor 2H-NbSe2. J Low Temp Phys 25:485–498

Werthamer NR, Helfand E, Hohenburg PC (1966) Temperature and purity dependence of the superconducting critical field, $H_{c2}$. III. electron spin and spin-orbit effects. Phys Rev 147:295–302

Woollam JA, Somacano RB, O’Connor P (1974) Positive Curvature of $H_{c2}$ versus $T_c$ boundaries in layered superconductors. Phys Rev Lett 32:712–714