Evolution of Kosterlitz-Thouless-Berezinskii (BKT) Transition in Ultra-Thin NbN Films

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Abstract. We explore the Berezinskii-Kosterlitz-Thouless (BKT) transition in ultrathin NbN superconducting films. We have measured the super fluid density ($n_s \propto 1/\lambda^2$), normal carrier density and resistivity ($\rho$) of a set of NbN thin films. Our results show that while the ground state is well described by BCS theory, at elevated temperatures, ultra-thin films show a sudden drop in superfluid density associated with the BKT transition close to the superconducting transition temperature ($T_c$). The sudden drop starts at a higher superfluid density than expected from the 2D XY model, which can be understood by considering the low vortex core energy and slight inhomogeneity in the system. Resistivity data is explained using effective medium theory (EMT) including both Aslamazov-Larkin and KT fluctuations. This is also in good agreement with the corresponding superfluid density.

1. Introduction

After the seminal work of Berezinskii-Kosterlitz-Thouless (BKT) [1] on 2D systems, a lot of effort has been made to understand the nature of BKT transition. It is a phase transition from quasi long range order to disordered phase in 2D and is expected to be universal in nature. The BKT transition plays a vital role in determining the superconducting properties (superfluid density, resistivity, Nernst effect, magnetization etc.) of a 2D superconductor including high-$T_c$ layered superconductors with weak interlayer coupling [2]. In these systems, the BKT transition can be studied through two different schemes. When approaching the transition from below, the superfluid density ($n_s$) is expected to go to zero discontinuously at the transition, with a "universal" relation between $n_s(T_{BKT})$ and $T_{BKT}$ itself. Approaching the transition from above, one can identify the BKT transition from superconducting fluctuations, which leaves its signature in the temperature dependence of various quantities such as resistivity, magnetization etc. In the second scheme, the information on the BKT transition is encoded in the correlation length $\xi(T)$, which diverges exponentially at $T_{BKT}$, in contrast to power-law dependence expected within Ginzburg-Landau (G-L) theory[3].

Within the 2D XY model originally investigated by Kosterlitz and Thouless both approaches should give identical information. However real superconductors have additional complications and always have some degree of inhomogeneity which tends to smear the sharp signatures of BKT transition compared to the clean case. Even when disorder in the system is homogeneous, the system shows an intrinsic tendency towards spatial inhomogeneity in the superconducting state [4], which has...
to be taken into account while analyzing the BKT transition. Apart from this, it has recently been argued that for a real superconductor the vortex core energy ($\mu$) can be very different from the value expected from 2D XY model. This can give rise to a completely different character of the vortex physics and even lead to a first order phase transition. Recently the relevance of the vortex core energy for the BKT transition has been theoretically explored in different context, ranging from the case of layered high-temperature superconductors to the one of superconducting interfaces in artificial heterostructures [5,8].

2. Experimental Details
To study the BKT physics in ultrathin conventional superconductor a series of epitaxial NbN thin films of thickness ranging from 3nm to 70nm were grown on (100) oriented MgO substrates by reactive dc magnetron sputtering, by sputtering a Nb target in Ar/N$_2$ (80:20) gas mixture at a substrate temperature of 600 °C. Details of sample growth and characterization have been reported in our earlier work [6]. The thickness ($d$) of the films was controlled by controlling the time of deposition keeping all other parameters constant. For films with $d>20$ nm, the thickness was measured using a stylus profilometer while for thinner films it was estimated from the time of deposition. The absolute value of magnetic penetration depth ($\lambda$) was measured using standard “two coil mutual inductance” technique [7] on 8mm diameter circular films prepared using shadow mask. The normal state carrier density ($n$) was deduced from Hall coefficient ($R_H$) measured on standard Hall bar geometry prepared by cutting a piece from the circular film. $R_H$ was calculated from reversed field sweeps from +12 to −12 T after subtracting the resistive contribution. The resistivity ($\rho$) at different temperatures were measured on the same films using a standard four-probe technique on 1mm width strips prepared using Ar ion beam milling. One advantage of our experiment is that for each thickness, we have measured the $n_s$, $R_H$ and $\rho$ on the same film.

3. Results and Discussion
Figure 1(a) shows mutual inductance ($M= M'+iM''$) between two coils as a function of temperature. The superconducting transition temperature ($T_c$) is extracted from the intersection of two tangents drawn above and below the transition on the $M'(T)$-$T$ curve. Figure 1(b) shows the variation of $T_c$ with film thickness from 13.37K for the 18nm film to 7.99K for the 3nm film. The reasonably narrow peak in $M''(T)$ curve show the very good quality of our films. The inset of figure 1(b) shows $n$ as a function of temperature. The room temperature carrier densities are scattered in a small range of values which shows that the films have similar stoichiometry [6].

Figure 2 shows the variation of $\lambda^{-2}(T) \propto n_s(T)$ and $\rho$ with temperature. For thinner films, we observe the deviation of $\lambda^{-2}(T)$ from BCS behavior closed to $T_c$. The jump in superfluid density close to $T_c$ becomes more and more prominent as we decrease the film’s thickness. This is a clear signature of the BKT transition. Within the BKT theory for 2D superconductors, $T_c$ is controlled by the proliferation

Figure 1. (a) This figure shows the mutual inductance ($M=M'+iM''$) between two coils for epitaxial NbN thin films. Solid lines correspond to $M'$ and dashed lines correspond to $M''$. (b) Shows the variation of $T_c$ with film thickness. The inset shows the normal ($n$) carrier density as a function of temperature.
of vortex-antivortex pairs which becomes entropically favorable at the temperature given by
\[ \frac{\pi J(T_{BKT})}{T_{BKT}} = 2 ; \]
where \( J(T) \) is the 2D superfluid stiffness. In the equation (1), \( J(T) \) is not only affected by the presence of quasiparticles above the superconducting energy gap but also by the presence of thermally excited vortex-antivortex pairs in the system. When the vortex core energy is large, the latter effect is negligible and \( T_{BKT} \) can be estimated from equation (1). However, in a BCS superconductor the vortex core energy is much lower than the value expected from the 2D XY model[5] and \( J(T) \) gets renormalized due to increase of bound vortex-antivortex pairs and \( T_{BKT} \) is further reduced from the mean field transition temperature \( T_{MF} \). To take into account the effect described above, we have numerically solved the renormalization group equations of the original BKT formalism [8] using only one free parameter: the ratio \( \mu/J(0) \), where \( J(0) \) is obtained from BCS fit to the experimental data (solid black line in fig 2.) as \( T \to 0 \). In any real system, the intrinsic inhomogeneity induced by disorder must be taken into account. To take into account the effect of inhomogeneity in \( J \), we average over the distribution of \( J(0) \); assuming a Gaussian distribution of relative width \( \delta \) for simplicity. The best fit values are listed in Table 1. Figure 2 shows that the above procedure leads to excellent fits although the ratio \( \mu/J(0) \) are small compared to the value, \( \mu/X_Y/J = \pi^2/2 = 4.9 \) expected from 2D XY model. The fact that in real material \( \mu \) is relatively smaller explains the observed downturn at higher superfluid density and lower temperature than the expected intersection of universal line \( 2T/\pi \) from 2D XY model.

To further establish our findings, we have analyzed our resistivity data by considering KT fluctuation and G-L fluctuation. In two dimensions, the contribution of SC fluctuation to conductivity can be encoded in the temperature dependence of SC correlation length, \( \delta \propto \xi^2(T) \). Due to proximity effect

Table 1 Magnetic penetration depth (\( \lambda(T\to 0) \)), \( T_{BKT} \), \( T_{MF} \) along with the best fit parameters obtained from KTB fits of the \( \lambda^2(T) \) and \( \rho(T) \) data for NbN thin films of different thickness. \( T_{MF} \) corresponds to the mean field transition temperature obtained from by extrapolating the BCS fit of \( \lambda^2(T) \) at \( T<T_{BKT} \).

| \( d \) (nm) | \( \lambda(0) \) (nm) | \( T_{BKT} \) (K) | \( T_{MF} \) (K) | From best fit of \( \lambda^2(T) \) | From best fit of \( \rho(T) \) |
|---|---|---|---|---|---|
| 3  | 582  | 7.77 | 8.3 | 1.19 | 0.108 |
| 6  | 438  | 10.85 | 11.4 | 0.606 | 0.048 |
| 12 | 403  | 12.46 | 1.8 | 0.457 | 0.027 |
| 18 | 383  | ---  | 13.37 | --- | --- |

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between the $T_{BKT}$ and $T_{MF}$, it is expected that most of the fluctuation regime will be accounted for G-L fluctuation while KT fluctuation will be relevant only between $T_{BKT}$ and $T_{MF}$. We interpolate between these two regimes using the Halperin-Nelson interpolation formula for the correlation length $\xi$,

$$\frac{\xi}{\xi_0} = \frac{2}{A} \sinh \left( \frac{b}{\sqrt{t}} \right)$$  \hspace{1cm} (2)

where $t=(T-T_{BKT})/T$ and A is a constant of order one. $b$ is the most relevant parameter and related to vortex core energy by $b \approx 2(4\mu_0 \sqrt{\kappa c} / \pi^2 J)$ [5], where $\kappa_c = (T_{MF}-T_{BKT})/T_{BKT}$ (The values calculated for $b$ using the best fit value of the superfluid density data is defined as $b_{theo}$ shown in Table 1.). The resistivity corresponding to the SC correlation length is given by

$$\frac{\rho}{\rho_N} = \frac{1}{1 + (\Delta \sigma / \sigma_0)} = \frac{1}{1 + (\xi / \xi_0)^2}$$ \hspace{1cm} (3)

To take into account the sample inhomogeneity we correlate the distribution of local superfluid stiffness used to analyze the superfluid density data below $T_{KTB}$ with distribution of local resistivity values $\rho=R/R_N$ according to equation (3), where local $T_{MF}$ is attributed to patch of having local superfluid stiffness $J_i$. The overall resistivity $\rho=R/R_N$ can be calculated using effective medium theory (EMT) where $\rho$ is the solution of the self consistent equation,

$$\sum w_i (\rho - \rho_i) \rho + \rho_i = 0\hspace{1cm} (4)$$

where $w_i$ is the occurrence probability of each resistor that we assume to be Gaussian as the local $J_i$ values. We apply the above procedure to analyze our resistivity data using the values of $T_{BKT}$ and $T_{MF}$ determined from the analyzed superfluid density data and A and b are taken as free parameters. The resulting fits are in excellent agreement with the experimental data shown in fig (2). All fitting parameters are listed in table (1). Considering that the interpolation formula is an approximation, the value of $b$ is in very good agreement with theoretically estimated value, $b_{theo}$.

4. Conclusion

In the present work, we have explored the nature of BKT transition in ultrathin NbN films. We have analyzed our superfluid density data using R-G analysis. Using the interpolation formula of the G-L fluctuations and BKT fluctuations, we have analyzed the resistivity data. The same set of parameters is used to analyze the superfluid density data and then resistivity data and it is found that both are in very good agreement with each other. We have shown that due to low vortex core energy, the down turn of the superfluid density starts at higher superfluid density value and lower temperature than expected in the 2D XY model, even though the universal character of the transition is preserved. We have observed that the ratio $\mu/J$ monotonically increases with decreasing film thickness, which will be discussed in details in our next publication.

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