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Effect of Te doping on superconductivity and charge-density wave in dichalcogenides 2H-$NbSe_{2-x}Te_x$ $(x = 0, 0.1, 0.2)$*

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Single crystals of Te-doped dichalcogenides 2H-$NbSe_{2-x}Te_x$ ($x = 0, 0.10, 0.20$) were grown by vapour transport method. The effect of Te doping on the superconducting and charge-density wave (CDW) transitions has been investigated. The sharp decrease of residual resistance ratio, RRR = R(300K)/R(8K), with increasing Te content was observed, indicating that the disorder in the conducting plane is induced by Te doping. Meanwhile the superconducting transition temperature, T_c, decreases monotonically with Te content. However, the CDW transition temperature, T_{CDW}, shown by a small jump in the temperature dependence of the resistivity near 30 K, increases slightly. The results show that the suppression of superconductivity might be caused by the enhancement of CDW ordering. The disorder has little influence on the CDW ordering.

Keywords: low-dimensional metal, superconductivity, charge-density wave, disorder
PACC: 7470J, 7430F, 7145L

1. Introduction

The compound 2H-$NbSe_2$ is a typical two-dimensional dichalcogenide which undergoes charge-density wave (CDW) transition at T_{CDW} of about 30 K and superconducting transition at T_c of 7.2K.[1] The coexistence of CDW and superconductivity and its mechanism have made it a research hotspot.[2,3] The possible mechanisms for the CDW instability include a simple Fermi surface (FS) nesting[4] or FS nesting with strong electron–phonon coupling effects[5,6] and a van Hove singularity or saddle point driven CDW.[7] Recently, two-band (two-gap) superconductivity in 2H-$NbSe_2$ has been suggested[2] and the enhanced Nernst effect in normal state which is interpreted by the ambipolar flow of two different types of charge carriers has been observed.[8] The nonmagnetic impurities in superconductors usually have only a mild influence on T_c, but they could cause a significant increase in H_{c2} as in the cases of NbTi and Nb_3Sn compounds. Such an impurity-induced enhancement in $H_{c2}(0)$ is theoretically shown to be even more effective in two-band superconductors because of the multiple scattering channels in two-band superconductors.[9] Impurities are also often used as effective vortex pinning centres to optimize the critical current in type-II superconductors.[10] Moreover, elemental substitution is a useful probe to detect the intrinsic factors that determine the interplay between superconductivity and CDW instability. Therefore, it is necessary and foremost to investigate elemental substitution effects in 2H-$NbSe_2$ to verify the theoretic predictions and find out appropriate approaches for optimizing superconducting properties.

In this paper we investigate the substitution effects of Te atoms on Se site in 2H-$NbSe_{2-x}Te_x$ (x =0,0.10,0.20) single crystals by measuring their structure and transport properties. The results show that the superconductivity is suppressed by the Te impurities and meanwhile the CDW ordering is even enhanced. The relationship between superconductivity and CDW is discussed.

2. Experimental

Single crystals with nominal composition of 2H-$NbSe_{2-x}Te_x$ (x =0, 0.1, 0.2) were grown by standard

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iodine vapour transport method. The growth details were reported previously.[11] Stoichiometric amounts of pure Nb (3N), Se (4N), and Te (4N) powders, together with a transport agent (iodine) were mixed together and placed in one end of a quartz tube, which was then evacuated and sealed. The sealed quartz tube was heated up in a temperature gradient furnace for one week. The charge-zone and growth-zone temperatures were 1073 K and 998 K respectively. Good quality platelets of single crystals were obtained.

The structure of the samples was confirmed by room-temperature x-ray diffraction (XRD) and the c-axis lattice parameter was calculated from the XRD patterns. A standard four- probe method was used to measure the in-plane resistivity. The transport property measurements were carried out in a Quantum Design PPMS-9 system.

3. Results and discussion

Figure 1 shows the XRD patterns of single crystals 2H-$NbSe_{2-x}Te_x$ ($x = 0, 0.1, 0.2$). All the peaks can be indexed by the hexagonal crystalline symmetry and are consistent with a 2H laminar structure. Only sharp ($00l$) diffraction peaks appear because the naturally cleaved surface is (001) plane. There are no other diffraction peaks besides ($00l$) peaks. The results indicate that the samples are indeed high-quality single crystals. The c-axis lattice constants calculated from the ($00l$) diffraction peaks are 12.53, 12.58, and 12.63 Å for x =0, 0.1, and 0.2 respectively. The c-axis lattice constant increases monotonically with Te content, which is consistent with the fact that the radius of Te ions is larger than that of Se ions.

The temperature dependence of the in-plane resistivity ρ_{ab} is shown in Fig.2. The inset shows the enlarged plots of ρ_{ab} versus T at low temperatures. The undoped 2H-$NbSe_2$ single crystal has a large residual resistivity ratio (RRR = R(300 K)/R(8 K)) of 25 and exhibits a very sharp superconducting transition at T_c of 7.2 K, implying that the sample is highly homogeneous. A clear jump just above 30 K in resistivity can be observed. Such a resistivity jump in this material is caused by CDW transition around T_{CDW} of 30 K,[12] which is usually only observed in the 2H-$NbSe_2$ samples with high RRR values (i.e., RRR $\geq$ 20).[11,13] As Te content increases, both T_c and RRR decrease quickly. RRR is an indication of disorder in the conducting plane. The decrease in RRR suggests that Te doping induces significantly disorder in the ab plane and Te impurities are effective scattering centres. T_c is 6.5, and 5.9 K for $x = 0.1$, and 0.2 respectively, while the transition width increases significantly as Te content increases. The results show that superconductivity is gently suppressed by Te doping. However, the resistivity jump around 30 K becomes more significant as Te content increases, and its onset temperature (T_{CDW}) increases slightly as well. This means that the CDW ordering is enhanced somewhat by Te substitution.

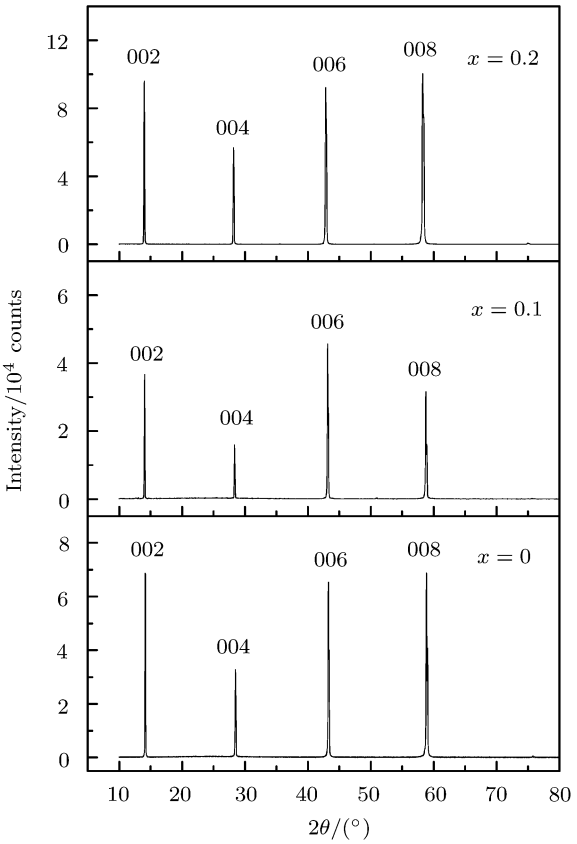


Fig.1. XRD patterns of single crystals 2H-$NbSe_{2-x}Te_x$ ($x = 0, 0.1, 0.2$).

Variations of the c-axis lattice constant, RRR, T_c, and T_{CDW} with Te content (x) are summarized in Fig.3. The variations of these physical parameters with Te content (x) are also listed in Table 1. It is easy to find that Te substitution has only a little influence on the c-axis lattice constant and T_{CDW}, but much influence on RRR. As shown in Fig.3, T_c decreases linearly with x, and a linear fitting produces a negative slope dT_c/dx of -6 K, which means that Te substitution on Se site results in suppression in T_c of only about 0.12 K for every 1% Te substitution. The estimated critical substitution concentration of Te to quench T_c completely is about 60

% of Te (please note that $x = 1$ should correspond to 50% substitution). The results are very different to the case where magnetic impurities like Fe are doped in 2H-$NbSe_2$. In Fe doped Fe_xNbSe_2, only 0.65% of Fe impurities ($x = 0.0065$) can suppress T_c down to less than 1 K, meanwhile the CDW ordering is also depressed simultaneously.[14] In our case, the non-magnetic Te substitution indeed causes significant disorder in the conducting plane, but T_c decreases slightly and CDW ordering is even enhanced somewhat. Te doping causes a slight increase in the c-axis lattice constant so that the coupling between the layers in 2H-$NbSe_{2-x}Te_x$ could become weaker and the system becomes more two-dimensional, which could account for the enhancement of the CDW instability.

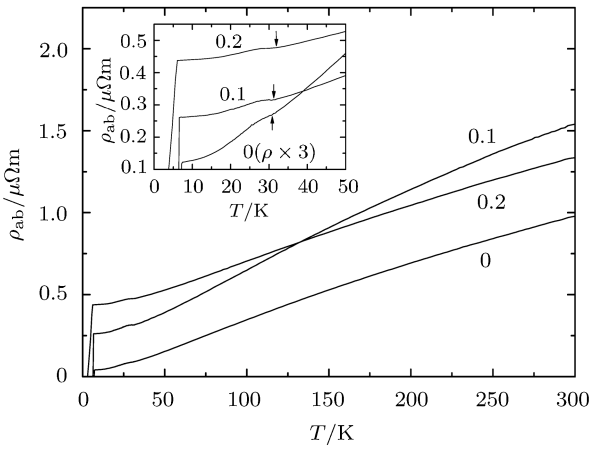


Fig.2. The temperature dependence of in-plane resistivity for $NbSe_{2-x}Te_x$ (x=0, 0.1, 0.2) single crystals. Inset: enlarged plot of ρ_{ab} vs. T for low temperatures. The arrows show the onset of the jumps in resistivity, which are caused by CDW transition.

According to Anderson's theorem, the conventional superconductivity is robust to the disorder caused by a small concentration of nonmagnetic impurities.[15] From Fig.3, it can be found that the decrease in T_c does not correlate with the decrease in RRR although both decrease with increasing Te content. There is a sharp drop of RRR at x =0.1 but T_c still decreases linearly and gently at $x = 0.1$. Therefore, we suggest that the decrease of T_c in this Te-substituted system might not result from the disorder scattering of Te-impurities. Actually, there is a competition between CDW phase and superconducting phase in this system. The enhancement of CDW ordering could cause a decrease of density of states at Fermi surface and thus suppress the superconductivity. Indeed, both T_{CDW} and the resistivity jump around T_{CDW} increase somewhat for Te-substituted samples, implying that there are more electrons condensed into CDW state. The CDW transition reduces the density of state at Fermi surface (because some portions of Fermi surface are removed by CDW gapping) so that superconductivity is suppressed. The interplay of CDW and superconducting orders has also been shown by a study on the effect of high pressure on CDW and superconductivity in this system.[16] It was observed that an increase in T_c with increasing pressure follows a decrease in T_{CDW}.[16] These results indicate that CDW phase and superconducting phase are the two competing phases, and there is an anti-correlation between them.

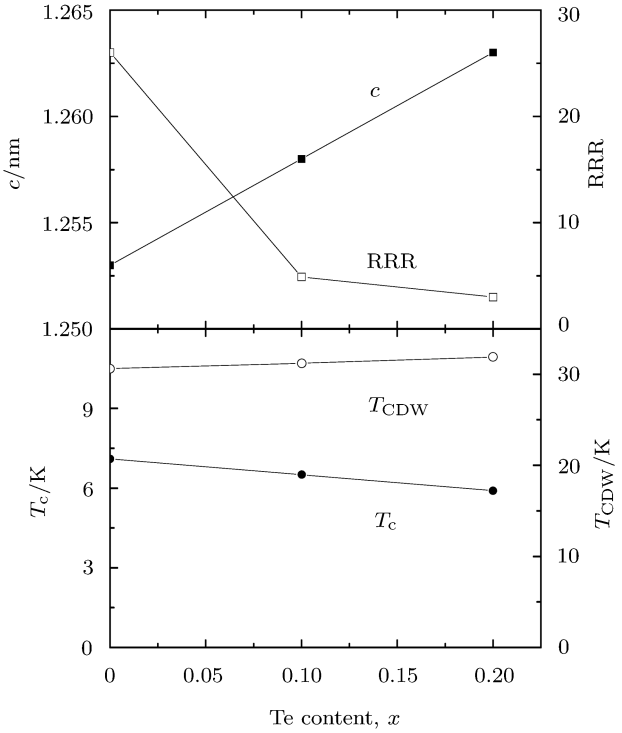


Fig.3. Variations of the c-axis lattice constant, RRR, T_c, and T_{CDW} with Te content (x).

Table 1. Variations of the c-axis lattice constant, residual resistance ratio (RRR), superconducting transition temperature (T_c), and CDW transition temperature (T_{CDW}) with Te content (x).

x	c/Å	RRR	T_c/K	T_{CDW}/K
0	12.53	25	7.2	30.6
0.1	12.58	4.9	6.5	31.2
0.2	12.63	3	5.9	31.9

4. Conclusion

In conclusion, we have successfully synthesized Te-doped 2H-$NbSe_{2-x}Te_x$ ($x = 0, 0.1, 0.2$) single crys-

tals and studied their structure, CDW transition and superconducting properties. Although both the RRR value and T_c decrease monotonically with increasing Te content and the disorder induced by impurity Te is remarkable, the influence of non-magnetic Te substitution on the superconducting properties is much weaker than the magnetic impurities like Fe. However, the CDW transition temperature increases slightly. We suggest that the decrease of T_c might mainly result from the enhancement of CDW ordering, and the pair-breaking effect of non-magnetic impurity Te scattering is very weak. The results imply that the superconducting state and CDW state are two competing orderings in this material.

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