Effect of pressure on a “111”-type iron pnictide superconductor


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The behavior of superconductivity of “111”-type iron pnictide superconductors, namely, LiFeAs, NaFeAs and LiFeP, is investigated at different pressures through electrical resistance measurements. For LiFeAs and LiFeP, the superconducting transition temperature $T_c$ decreases monotonously with increasing pressure, with the pressure coefficient of $dT_c/dP$ being $-1.38$ and $-1.26$ K/GPa, respectively. The $T_c$ of NaFeAs increases to a maximum value with the pressure increasing to 3 GPa; further increasing the pressure suppresses $T_c$ with the slope of $dT_c/dP$ about $-3.40$ K/GPa.

Keywords: iron-based superconductor; “111” system; high pressure

1. Introduction

The newly discovered iron pnictide superconductors have attracted enormous attention for their high superconducting transition temperature. These iron pnictide compounds can be classed into three types: (i) “1111”-type ROFeAs (R = rare earth metal or alkaline-earth metal) [1–6], (ii) “122”-type AeFe$_2$As$_2$ (Ae = alkaline earth metal) [7] and (iii) “111”-type AFeAs(P) (A = Li, Na) [8–10]. These compounds have a layered structure with a stack of alternating iron-pnictide and charge reservoir layers. The technique of high pressure has played a role in exploring new other iron-based superconductors and studying the superconducting mechanism [11–18]. Soon after the discovery of superconductivity in LaO$_{1-x}$F$_x$FeAs with $T_c$ ∼ 26 K [1], applying external pressure on the superconductor enhances $T_c$ up to 43 K [11]. There is a spin density wave (SDW) transition in most of these undoped or slightly doped iron-based compounds. External pressure can suppress SDW transition and induce superconductivity, which is similar to the role of chemical doping. For LaFeAsO and BaFe$_2$As$_2$ compounds, the SDW transition happens at about 150 and 140 K, respectively. When an external pressure is applied, the SDW transition temperature $T_{SDW}$ goes down and superconductivity subsequently emerges [13,15]. When $T_c$ is pushed to a maximum value with pressure, it decreases at higher pressures. However, for doped RFeAsO$_{0.85}$ (R = Sm and Nd) [12], $T_c$ is suppressed monotonously with increasing pressure. It seems that the behavior of $T_c$ tuned by pressure is complex. In this work, we report the effect of pressure on the $T_c$ of “111”-type superconductors.
2. Experimental methods

The samples of LiFeAs, NaFeAs and LiFeP were synthesized by the solid-state reaction method described elsewhere [8,10]. The pressure-induced evolution of the superconducting transition for LiFeAs and NaFeAs was investigated by four-probe electrical resistance measurement methods in a diamond anvil cell. The pressure was measured at room temperature by the ruby fluorescence method before and after each temperature cooling down. For the LiFeP sample, a double-layer piston cylinder-type pressure cell was used [19]. Silicone oil served as the pressure-transmitting medium. The pressure was determined at low temperatures by monitoring the pressure-induced shift of the superconductive transition temperature of Pb placed close to the sample.

3. Results and discussion

The “111”-type iron-based superconductors are crystallized into a Cu₂Sb-type structure with $P\bar{4}/nmm$ symmetry, as shown in Figure 1. In the layered structure, iron pnictide and a Li or Na layer are stacked alternately. Fe atoms are in a four-fold coordination, forming a FeAs(P)₄ tetrahedron. Table 1 shows the parameters of these crystal structures. The crystal lattice parameters

![Crystal structure for “111”-type iron-based superconductors.](image)

Table 1. Crystal structure parameters for “111”-type superconductors under ambient pressure and room temperature.

<table>
<thead>
<tr>
<th></th>
<th>a (Å)</th>
<th>c (Å)</th>
<th>$\alpha^\circ$</th>
<th>$\beta^\circ$</th>
<th>Anion height (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LiFeAs</td>
<td>3.776</td>
<td>6.358</td>
<td>102.8</td>
<td>112.9</td>
<td>1.51</td>
</tr>
<tr>
<td>NaFeAs</td>
<td>3.949</td>
<td>7.039</td>
<td>108.3</td>
<td>110.1</td>
<td>1.43</td>
</tr>
<tr>
<td>LiFeP</td>
<td>3.692</td>
<td>6.031</td>
<td>108.6</td>
<td>109.9</td>
<td>1.33</td>
</tr>
</tbody>
</table>

Note: *$\alpha$ and $\beta$ denote the two-fold and four-fold bond angle of the FeAs(P)₄ tetrahedron, respectively.*
of LiFeP are the smallest among the three “111” compounds. The bond angle for a regular tetrahedron is about 109.47°. From Table 1, we can see that for both NaFeAs and LiFeP, the FeAs(P)₄ tetrahedron approaches the regular one, while the FeAs₄ tetrahedron for LiFeAs shows elongation along the c-axis, which leads to a much smaller As–Fe–As (two-fold) angle and a larger anion height from As atom to Fe plane than that of NaFeAs.

Figure 2. Temperature dependence of electrical resistance under different pressures for (a) LiFeAs, (b) NaFeAs and (c) LiFeP.
Figure 2(a)–(c) shows the temperature dependence of electrical resistance under different pressures for LiFeAs, NaFeAs and LiFeP, respectively. For LiFeAs and LiFeP, \( T_c \) decreases monotonously with increasing pressure, while the \( T_c \) of NaFeAs increases to a maximum value as pressure increases to 3 GPa; further increasing the pressure suppresses \( T_c \). The superconducting transition of NaFeAs at ambient pressure is broad, which is also observed by another group \[20\]. However, it is surprising that the transition becomes sharper with initial increasing pressure. This is probably related to the reactive nature of the NaFeAs sample.

The curves of pressure dependence of \( T_c \) for the three superconductors are drawn in Figure 3, where we use \( T_c^{\text{onset}} \) value for NaFeAs and LiFeAs and \( T_c^{\text{zero}} \) value for LiFeP. The figure clearly shows the different characters of \( T_c \) tuned by pressure for “111”-type iron-based superconductors. Similar to the behavior of pressure tuning \( T_c \) for SmFeAsO\(_{0.85}\) and NdFeAsO\(_{0.85}\), pressure suppresses \( T_c \) monotonously with a pressure coefficient of \(-1.38\) K/GPa and \(-1.26\) K/GPa for LiFeAs and LiFeP, respectively. As for NaFeAs, the pressure coefficient is positive at the initial increasing pressure stage. \( T_c \) increases as the pressure increases from ambient pressure to 3 GPa, followed by a quick decrease at higher pressures, with the slope of \( dT_c/dP \) about \(-3.4\) K/GPa. The maximum \( T_c \) of 31 K is observed at about 3 GPa. This parabolic pressure dependence of \( T_c \) is also observed in LaFeAsO\(_{1-x}\)F\(_x\) and AFe\(_2\)As\(_2\) (A = Sr, Ba).

For iron pnictide superconductors, the [FeAs(P)] layer is considered as the superconducting path. Therefore the crystal chemistry parameters, such as the Fe–As bond length or the As(P)–Fe–As(P) bond angle, are critical to superconducting transition temperatures. Mizuguchi et al. \[21\] established the plot of \( T_c \) dependence on the anion height for the typical Fe-based superconductors. The plotted data points exhibit a unique curve with a peak around 1.38 Å. \( T_c \) would decrease when the anion height deviates from the peak value. Furthermore, the plot includes LiFeAs and NaFeAs studied in this work, while the data under high pressures for NdFeAsO\(_{0.85}\), SrFe\(_2\)As\(_2\), BaFe\(_2\)As\(_2\) and FeSe also match well with the curve. Mito et al. \[17\] reported the structure evolution of LiFeAs under pressure up to 17 GPa. The As–Fe–As (two-fold) angle and the Fe–As bond length decrease with increasing pressure. Although the relation between anion height and pressure was not given in that paper, with the data of angle and bond length at different pressures it can be deduced. The anion height can be obtained by the formula: \( h = d \times \cos(\alpha/2) \), where \( h \) is the anion height, \( d \) the Fe–As bond length and \( \alpha \) the As–Fe–As (two-fold) angle. It is found that the anion height increases with pressure. According to this point of view, we suppose that the anion height...
for NaFeAs decreases with the initial increasing pressure and then increases at higher pressures. If this is true, it can well explain the behavior of \( T_c \) tuned by pressure, as its anion height at ambient pressure is also larger than the optimized value of 1.38 Å.

As for LiFeP, the anion height is 1.33, very close to the optimized value, but its \( T_c \) is much lower. This is likely caused via the more extended electronic structure of phosphide over arsenide. LiFeP and LiFeAs have similar tendencies of \( T_c \) tuned by pressure and their pressure coefficients are close. Additionally, \( T_c \) and crystal lattice constants \( a \) and \( c \) for LiFeP at ambient pressure and LiFeAs at 5.5 ~ 6.5 GPa become comparable [19]. Therefore, we can view LiFeP as a compressed LiFeAs.

4. Conclusion

In summary, we have studied the effect of pressure on the “111”-type superconductors. There are two behaviors of \( T_c \) tuned by pressure. For LiFeAs and LiFeP, \( T_c \) decreased monotonously with increasing pressure. For NaFeAs, \( T_c \) is enhanced by pressure up to a maximum of 31 K at about 3 GPa before decreases at higher pressure.

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References

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