What will be the maximum $T_c$ in the iron-based superconductors?

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Using the newly developed real space vortex-lattice based theory of superconductivity, we study the maximum superconducting transition temperature ($T_c^{max}$) in the iron-based superconductors. We argue that the $c$-axis lattice constant plays a key role in raising the $T_c^{max}$ of the superconductors. It is found that all the reported FeAs superconductors can be divided into two basic classes ($c/a \approx 3$ and $c/a \approx 5/2$) depending on the lattice constants, where $a$ is the Fe-Fe distance in the $xy$-plane and $c$ is the Fe-Fe layer distance along the $z$-axis. Our results suggest that the former class has a maximum $T_c^{max} < 60$ K, while the latter class has a lower $T_c^{max} \leq 40$ K. Our investigations further indicate that, in order to enhance $T_c^{max}$ in this family of compounds, new class of superconductors with a larger ratio of $c/a$ should be synthesized. It is likely that their $T_c^{max}$ values could be raised into the liquid nitrogen range (77 K) and 100 K, supposing the new analogues with $c/a \approx 5$ (approximately $c > 13 \AA$, if $a = 2.750 \AA$) and $c/a \approx 11$ ($c > 31 \AA$) can be experimentally achieved, respectively.

For the new FeSe series, our mechanism predicts that their $T_c^{max}$ is impossible to exceed 30 K due to a relatively shorter $c$-axis lattice constant ($c/a \approx 2$). Finally, based on the new experimental results [arXiv:0811.0094] and [arXiv:0811.2205], the possible ways to raise the $T_c$ of the iron-based superconductors into 70 K are also suggested.

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I. INTRODUCTION

Since the discovery of superconductivity at $T_c = 26$ K in the iron-based LaO$_{1-x}$F$_x$FeAs [1], great efforts have been devoted to explore new kind of iron oxypnictide superconductors with the higher superconducting transition temperature. As shown in Fig. 1 through elemental substitution, $T_c$ was drastically raised to 43 K ($> 39$ K, the commonly assumed McMillan Limit) in SmO$_{1-x}$F$_x$FeAs [2] that can be defined as an unconventional superconductor. One day later, superconductivity at 41 kelvin in another iron-based layered compound CeO$_{1-x}$F$_x$FeAs [3] was reported. Immediately, many group reported that the $T_c$ could be further increased to above 50 K, for example, 52 K in PrO$_{1-x}$F$_x$FeAs [4], 55 K in SmO$_{1-x}$F$_x$FeAs [5] and 56 K in Gd$_{1-x}$Th$_x$FeAsO [6]. Facing the rapid increase of $T_c$, researchers and the media have become too crazy about the new discovery [7]. This situation is remarkably similar to that of the discovery of cuprate superconductors in 1986. Some researchers even claimed that the new discovery may pave the way for the development of superconductors that can operate at room temperature [8].

The quest for higher $T_c$ iron-based superconductors is still continuing. For all researchers, it is not known to what extent $T_c$ can increase in these materials. However, on 29 August, we argued that the superconducting transition temperature of the previously reported series compounds is difficult to break through $T_c = 60$ K [9]. Later, Steele concluded that since the metallic bond (conduction band) in the material is confined to the lines of iron atoms, the $T_c$ of any of these materials will never be as high as in the high-$T_c$ cuprates [10]. Now, more than two months have passed since our prediction that these materials could be adjusted by a appropriate charge carrier density to raise theirs $T_c$ by a few more kelvins. Since

\begin{figure}
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{The schematic plot of the discovery of iron-based superconductors in 2008. We argue that all the reported FeAs superconductors can be divided into two basic classes (large $c$-axis and short $c$-axis), and the corresponding $T_c$ values are very difficult to exceed 60 K.}
\end{figure}
then, though several new superconductors have been discovered [11, 12, 13, 14, 15, 16, 17, 18], their \( T_c \) are also lower than 60 K (see Fig. 1) as our suggested.

Some readers are eager to know how can we make such a bold prediction (the \( T_{c\text{max}} \) of the related materials has to be less than 60 K)? In the present paper, on the one hand, we try to answer the question raised above. On the other hand, the ways how to achieve some higher \( T_c \) iron-based superconductors are suggested.

II. WHY WE NEED A FRESH THINKING TO UNDERSTAND SUPERCONDUCTIVITY?

Superconductivity was used to be considered as a peculiar physical phenomenon, which can only be observed in few special materials (or elements). Now, as more and more materials (more than several thousands) with different structures and physical properties have been discovered to exhibit superconductivity, the previous viewpoint must be changed. In our opinion, it is most likely that any crystalloid materials with a appropriate charge carrier density (not too high, not too low) may found to be the superconductors under an appropriate temperature. In fact, the field of superconductivity is in a transition from an old era [Which materials (or elements) can be a superconductor?] to a new era [Which materials (or elements) cannot be a superconductor?]. Therefore, it is unnecessary to be too excited about the observation of the superconductivity in layered iron arsenic compounds.

In the past century, the experimental scientists have discovered so many different kinds of superconductors, which greatly challenge the thinking of the theoretical physicists. What causes the superconductivity? For most “theoretical physicists”, it seems natural that different superconductors will work differently, or we always need a new mechanism for a new superconductor. To speculate the mechanisms for the various superconductors, they have spend a good deal of time using computers to compute numerical solutions to equations obtained by the complicated mathematical derivation. They mistakenly believe that the reliable results can only be expected by the applying of high-complex mathematics and advanced computer. We think this approach must be given up. It is time for us to realize that God didn’t create superconductivity in such a complicated way as people considered to be. We believe that the superconductivity, as a common phenomenon in nature, its law should be intrinsically simple and deterministic [19]. It is physically unrealistic to expect that the maths and computer can unravel the superconductivity mystery and tell us the right answer. In fact, the misuse of the mathematical and computing techniques rather than physics thinking may obscure the essential physics underlying the superconducting phenomenon.

Figure 2 shows the unit cell of three typical superconductors, they are (a) the conventional superconductor Nb with a bcc structure, (b) the iron-based LaO\(_{1-x}\)F\(_x\)FeAs and (c) the cuprate Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_8\) for the conventional superconductors, the mainstream physicists still believe that the BCS theory [20] can explain the behavior of superconductivity. For the cuprate high-\( T_c \) superconductors [21], a widely-accepted explanation is still missing despite great effort since 1986. Recently, Anderson [22] even pointed out that the need for a bosonic glue (phonon) in cuprate superconductors is folklore rather than the result of scientific logic and many theories about electron pairing in cuprate superconductors may be on the wrong track. For the new iron-based superconductors, some researchers believe that the new family contains new mysteries and some new theoretical models should be invented.

Even though the BCS theory has been proved to be invalid in most of the known superconductors, this situation has not made researchers rethink one basic question: Is the BCS theory correct? Most recently, I have discussed with Prof. Anderson about the reliability of BCS theory [23]. He considered the application of the BCS theory of superconductivity should be confined within a small domain of materials, the polyelectronic metals. But, I have showed clearly that the phonon-mediated BCS theory is fundamentally incorrect (see Section II of Ref. [19]). I insisted that the BCS theory is unsuitable not only for the non-conventional superconductors but also for the conventional superconductors.

It is well known that the BCS theory was established on the basis of quantum mechanism, which is extreme sensitivity to a small perturbation of the Hamiltonian of the studied system. One can recall the process of the establishment of the BCS theory, even for the simplest
superconductor of Fig. 2(a), which included a large number of man-made physical hypotheses and mathematical approximations (most of which are physically unreasonable). It is no doubt that, for the complex superconductors of Figs. 2(b) and (c), the quantum mechanics is powerless. We have to give up the original idea and procedure of BCS type, of course, the new theory of superconductivity should not be too concerned about the specific atomic structures of the superconductors.

III. THEORY

Physically, the superconducting state is merely a charge-order phase in the superconductors. It is unwise to endow superconductivity with too many mysterious elements. In the framework of BCS theory, the charge carriers are assumed to be in $k$-space (dynamic screening) order but $r$-space (real-space screening) disorder. From a strictly mathematical viewpoint, $k$-space picture and $r$-space picture are tightly correlated, obviously, the BCS picture is unwarranted conjecture in both physics and maths. We argue that a reasonable superconducting theory must be mathematically self-consistent, in other words, the charge carriers should display a similar degree of order in both $k$-space and $r$-space. In addition, we believe that a physical theory in real-space picture is naturally more reliable than that in momentum-space picture, as all physical phenomena take place in the real space rather than the imaginary $k$-space.

Recently, we have developed a real space vortex-lattice based theory of superconductivity which can naturally explain some complicated problems in conventional and non-conventional superconductors, included the new iron arsenide superconductors [9, 19, 24, 25, 26, 27, 28]. As shown in Fig. 3(a), the mechanism contains two main factors: the framework structure (black lines) of atoms and the vortex lattice (red lines) of the charge carriers (electrons). In this case, a real space long range magnetic order (vortex line, or stripe) and superconductivity coexist to form a dimerized charge supersolid (a charge-Peierls dimerized transition), as seen in Fig. 3(b).

In the previous studies [9, 19, 27], we argued that the physically significant critical value for the most stable vortex lattice is that at which a uniform distribution of vertex lines in the plane perpendicular to the stripes. In this sense, two low-temperature tetragonal phases (LTT1 and LTT2) and two simple hexagonal phases (SH1 and SH2) might be the ideal candidates for the stable charge-stripe order of paired electrons, as shown in Fig. 4.

For a doped superconductor, the charge carrier doping level $x$ is given by

$$x = p(h, k, l) = 2 \frac{V_{abc}}{V_{ABC}} = 2 \times \frac{1}{h} \times \frac{1}{k} \times \frac{1}{l},$$ (1)
and the corresponding charge carrier density is
\[ \rho_s = \frac{2}{ABC} = \frac{2}{hkl}abc = \frac{x}{abc}. \]

where \((A, B, C) = (ha, kb, lc), h, k,\) and \(l\) are integral numbers, and \(V_{abc}\) and \(V_{ABC}\) are the unit cell volumes of the lattice and the corresponding superlattice, respectively.

It should be pointed out that, for most actual superconducting materials, their superconducting vortex lattices are likely in some not standard vortex structures with some degree of distortion compared to the standard structures of Fig. 4. Obviously, the distortion of the vortex lattice can affect the stability of the superconducting state, at the same time decrease the superconducting transition temperature of the corresponding superconductor. Experimentally, by exerting an external pressure on the superconductor, or through the substitution of smaller ions (chemical inner pressure), the vortex lattice distortion can be corrected in some extent, as a result, increasing the \(T_c\) of the studied superconductor. These effects imply that the shrinking of the lattice constants may enhance the \(T_c\) of the superconductor.

But in the following discussions we will show that increasing the \(c\)-axis lattice constant can result in a much more intensive enhancement of \(T_c\) in the iron-based superconductors. It must be pointed out that these two conclusions are not contradictory. Just as in the cuprate superconductors, although it has been proven that the reducing of the lattice constants by an external pressure through is probable resulting in the increasing of the \(T_c\) in these superconductors, however it is no doubt that the most effective means of enhancing \(T_c\) is by means of increasing \(c\)-axis lattice constant of the superconductors. As we can see that the \(T_c\) of the cuprate superconductors had been raise easily from the \(T_c = 40\) K of the La\(_{2−x}\)Ba\(_x\)CuO\(_4\) (\(c = 13.2\) Å), to \(T_c = 80\) K of the YBa\(_2\)Cu\(_3\)O\(_4\) (\(c = 27.24\) Å), \(T_c = 110\) K of the Bi\(_2\)Sr\(_2\)Ca\(_2\)Cu\(_3\)O\(_{10}\) (\(c = 37.1\) Å) and \(T_c = 136\) K of the HgBa\(_2\)Ca\(_2\)Cu\(_3\)O (\(c = 158.3\) Å). The potential physical reasons behind these results are still unclear.

According to Fig. 5, the \(T_c\) of a superconductor is directly proportional to the stability of the superconducting vortex lattice phase. There are three factors (temperature, charge carrier density and \(c\)-axis lattice constant) that affect vortex lattice’s situations, which in turn influence the \(T_c\) of a superconductor. Each of these influences will be discussed in greater detail in the following subsections.

A. The influence of temperature on the \(T_c\)

In the ideal situation of absolute zero temperature, the vibration of the lattice framework and the fluctuation of the vortex lines (stripes) can be neglected, as shown in Fig. 5(a). In this special case, the vortex lattice is in the most stable minimum energy superconducting state (the so-called ground state). When \(T_1 > 0\), there exist inevitably the vibration of the lattice framework and the fluctuation of the vortex lines, as shown in Fig. 5(b). Furthermore, these may directly lead to a stronger stripe-stripe interaction due to a shorter minimum stripe-stripe distance (\(\xi_1 < \xi_0\)). As illustrated in Fig. 5(c), the stripe-stripe interaction increased with the increasing of the temperature \((T_2 > T_1)\). These discussions imply that temperature on the impact of the superconducting transition temperature \(T_c\) is always negative and the lattice vibration (phonon) is impossible to provide the “glue” for the superconductors.
superconducting transition temperature of iron-pnictide high-temperature superconductors, their charge carrier density on the

FIG. 6: The schematic interpretation of the influence of B. The influence of charge carrier density on the density.

superconducting phase due to the excessive charge carrier concentration on the fundamental properties of high-Tc superconductors has been experimentally and theoretically studied by many investigators. Scientists have not yet reached a consensus on this issue.

It is well known that, in both the cuprate and the new iron-pnictide high-temperature superconductors, their superconducting transition temperature $T_c$ can be modified by the charge carrier density $p_s$ (or the doping level $x$). So far, though the influence of the carrier concentration on the fundamental properties of high-$T_c$ superconductors has been experimentally and theoretically studied by many investigators. Scientists have not yet reached a consensus on this issue.

In our theoretical framework of Fig. 3, the relationship between the charge carrier density and $T_c$ is very simple and intuitive. As shown in Fig. 6, in a low doping superconducting vortex phase of Fig. 6(a), the nearest neighbor distance ($\xi_1$) between the vortex lines is large, so that the stripe-stripe interactions are weak and the superconductor is expected to have a higher $T_c$. When further charge carriers are added to the superconductor, the vortex lines [see Fig. 6(b)] become more crowded than that of Fig. 6(a) ($\xi_2 < \xi_1$). As a result, a higher charge-carrier density will produce a stronger interaction among the vortex lines and consequently lead to a lower $T_c$. Figure 6(c) shows an extreme case (with the doping level $x = 2$) in which each unit cell contains two electrons, obviously, the superconducting vortex lattice no longer exists due to the great enhancement of the stripe-stripe interactions. These result strongly suggest that a superconducting phase can be destroyed easily by the extra charge carriers in a superconductor. We consider the picture of Fig. 6(c) provides a vivid interpretation: Why the good conductors (Cu, Au, and Ag) and overdoped high-$T_c$ superconductors do not achieve or exhibit superconductivity? In brief, the superconducting state is characterized by a real-space periodic vortex lattice while the non-superconducting state is dominated by the anomalous distribution of charge carriers.

C. The influence of c-axis lattice constant on the $T_c$

For the cuprate superconductors, there are many experimental facts showing a strong dependence of the maximum superconducting transition temperature ($T_c^{\text{max}}$) on the c-axis lattice constant. Normally, a superconductor with a larger c-axis lattice constant may have a higher maximum superconducting transition temperature. But the dependency of $T_c^{\text{max}}$ on the a-axis (or b-axis) lattice constant is much less sensitive compared to that of the c-axis lattice constant.

Here, we try to uncover the possible relationships between the lattice constant $c$ and $T_c^{\text{max}}$ based on the scenario in Fig. 4. Suppose there are two different kinds of superconductors with the lattice constants $(a, b, c_1)$ and $(a, b, c_2 = 2c_1)$ respectively, as shown in Fig. 7. If $c_1 = 2\sqrt{3}a$, some hexagonal vortex lattices can be formed in the superconductors at some appropriate doping levels $x = 1/2, 1/8$ and 1/4, which are shown in Figs. 7(a), (b) and (c) respectively. As can be seen from the figures, all the superconducting layers are doped in the cases of Figs. 7(a) and (c), it is clear that the former case (for the superconductor having a shorter c-axis parameter) will exhibit a lower $T_c$ due to a much stronger stripe-stripe interaction among the crowded vortex lines. Of course, by reducing the charge carrier concentration in the superconductor of Fig. 7(a), it is possible that the two superconductors could have the same charge carrier density, are shown in Figs. 7(b) and (c). It should be noted that only half of the superconducting layers are doped in Fig. 7(b). This inevitably lead to the escape-ment of electrons from the vortex lines to the undoped layers, as illustrated in Fig. 7(b), consequently, decreases the stability of the superconducting vortex lattice and reduces the corresponding superconducting transition temperature. For a even shorter c-axis lattice constant, for...
FIG. 7: An explanation why a layered material with a large $c$-axis lattice constant tends to be a high-$T_c$ superconductor. (a) A crowded superconducting vortex lattice in a superconductor with a short $c$-axis lattice constant, the corresponding $T_c$ is low due to a stronger stripe-stripe interaction among the vortex lines. (b) A relatively uncrowded vortex lattice in the short $c$-axis superconductor, though the stripe-stripe interactions could have been reduced greatly, the stability of the superconducting vortex lattice may be decreased by some mis-site electrons. (c) A possible higher $T_c$ superconducting vortex lattice in a larger $c$-axis superconductor.

Thus raising $T_c$ of the superconductor.

It is apparent from the above discussions that a material with a larger $c$-axis lattice constant could potentially be a high-temperature superconductor. This does not mean that the $T_c$ can increase unboundedly by the increasing of the $c$-axis lattice constant of the superconducting material. In our mechanism of superconductivity, it is not difficult to find that a appropriate stripe-stripe interaction is absolutely necessarily for the formation of the superconducting vortex lattice.

D. The critical energy of the superconductor

In this subsection, from the viewpoint of energy, we elaborate on the relationship between the stability of superconducting vortex phase and the two physical parameters (temperature $T$ and lattice constant $c$). Physically, the stability of one superconducting phase will decrease with the increase of the superconductor’s energy. In subsection III it had been shown that the temperature remained uncondutive to the formation of the superconducting vortex state. This conclusion can be expressed simply by

$$E_T = \alpha T,$$

where $E_T$ denotes the temperature-dependent energy of the vortex lattice, $T$ is the temperature and $\alpha$ is a structure and material-related parameter.

Similarly, the results of the discussions in Subsection III B and Subsection III C can be explicitly presented as follows

$$E_S = \beta \frac{1}{c},$$

where $E_S$ denotes the (charge carrier density and $c$-axis lattice constant)-dependent energy of the vortex lattice, $c$ is the $c$-axis lattice constant and $\beta$ is another material-related parameter. Combining Eqs. (3) and (4) yields the total energy $E(T, c)$ of the vortex lattice

$$E(T, c) = E_T + E_S = \alpha T + \beta \frac{1}{c}.$$  

Let $T_c$ be the superconducting transition temperature, then we can define the critical energy of the superconductor as

$$E_C = E(T_c, c) = \alpha T_c + \beta \frac{1}{c},$$

here we assume that the $E_c$ value is same for any superconductors. And the superconducting vortex phase should satisfy the following criterion

$$E(T, c) - E(T_c, c) \leq 0,$$

while for the non-superconducting phase, we have

$$E(T, c) - E(T_c, c) > 0.$$

In the following sections, we will apply the above general analysis to the specific iron-based superconductors.
TABLE I: Experimental data of $T_c$, lattice constants ($a$ and $c$) and $c/a$ ratio for the iron-based superconductors with $c/a \approx 3$, where $a (= a_0/\sqrt{2})$ is the nearest-neighbor Fe-Fe distances.

| Superconductors | $a$(Å) | $c$(Å) | $c/a$ | $T_c$(K) |
|-----------------|--------|--------|--------|----------|
| [1]LaO$_1$-xF$_x$FeAs | 2.850 | 8.739 | 3.066 | 26 |
| [2]SmO$_1$-xF$_x$FeAs (x = 0.15) | 2.786 | 8.496 | 3.050 | 43 |
| [3]CeO$_1$-xF$_x$FeAs (x = 0.16) | 2.820 | 8.631 | 3.061 | 41 |
| [4]PrO$_1$-xF$_x$FeAs (x = 0.11) | 2.818 | 8.595 | 3.050 | 52 |
| [5]SmO$_1$-xF$_x$FeAs (x = 0.1) | 2.768 | 8.428 | 3.045 | 55 |
| [6]Gd$_{1-x}$Th$_x$FeAsO (x = 0.2) | 2.769 | 8.447 | 3.054 | 56 |
| [12]Th$_{1-x}$Th$_x$FeAsO (x = 0.2) | 2.759 | 8.412 | 3.049 | 50 |
| [15]TbFeAsO$_{0.85}$ | 2.750 | 8.376 | 3.046 | 42 |
| [20]SmO$_1$-xF$_x$FeAs (x = 0.35) | 2.778 | 8.522 | 3.068 | 52 |
| [29]GdO$_1$-xF$_x$FeAs (x = 0.17) | 2.829 | 8.650 | 3.058 | 50.6 |
| [31]SmO$_1$-xF$_x$FeAs (x = 0.3) | 2.777 | 8.482 | 3.054 | 54.6 |
| [32]SmO$_1$-xF$_x$FeAs (x = 0.2) | 2.775 | 8.481 | 3.056 | 54 |
| [33]SmFeAsO$_{1-x}$ (x = 0.15) | 2.756 | 8.407 | 3.050 | 55 |
| GdFeAsO$_{1-x}$ (x = 0.15) | 2.760 | 8.453 | 3.063 | 53.5 |
| NdFeAsO$_{1-x}$ (x = 0.15) | 2.788 | 8.521 | 3.056 | 53.5 |
| PrFeAsO$_{1-x}$ (x = 0.15) | 2.806 | 8.566 | 3.053 | 51.3 |
| CeFeAsO$_{1-x}$ (x = 0.15) | 2.814 | 8.605 | 3.058 | 46.5 |
| LaFeAsO$_{1-x}$ (x = 0.15) | 2.844 | 8.707 | 3.062 | 31.2 |
| [16]Sr$_{1-x}$La$_x$FeAsF | 2.826 | 8.961 | 3.171 | 36.1 |
| [18]Sr$_{1-x}$Sm$_x$FeAsF (x = 0.5) | 2.825 | 8.961 | 3.172 | 56 |

IV. THE MAXIMUM $T_c$ IN THE IRON-BASED SUPERCONDUCTORS

Up to now, there are about dozens of iron-based superconductors have been reported. Based on our mechanism of superconductivity, these superconductors can be divided into two basic classes ($c/a \approx 3$ and $c/a \approx 5/2 = 2.5$) according to the $a$-axis lattice constants. It will be shown that the $c/a \approx 3$ class has a higher $T_c$ than that of the $c/a \approx 5/2$ class due to a larger $a$-axis lattice constant in the former class.

Table I shows the experimental data of $T_c$, lattice constants ($a$ and $c$) and $c/a$ ratio of the majority reported iron-based superconductors. It should be noted that in this paper the lattice constant $a (= a_0/\sqrt{2})$ is the Fe-Fe distance in the $xy$-plane (the superconducting plane). It is easy to find that, except the last two samples, all the compounds have a similarity $c/a$ value of 3. According to the value of $c$-axis lattice constants, the other reported iron-based superconductors can be classified into another class, as shown in Table II. In the previous paper [28], we have mentioned that the $c$-axis lattice constant of the Fe$_2$As$_2$ family should be redefined as $c = c_0/2$, where $c_0$ is the corresponding experimental value of the $c$-axis lattice constant. It is apparent from this table that all the $c/a$ values are very close to 2.5.

The relationships between the $c$-axis lattice constants and $T_c$ are depicted in Fig. 5 for both classes. Let us look at Figs. 5(a) of $c/a \approx 3$ class, the blue curve indicates that the maximum $T_c$ of this group is difficult to exceed 60 K. In addition, there are two exceptional values, as marked in the subfigure, which are most likely to belong to a new class of $c/a \approx 16/5$. For the $c/a \approx 5/2$ class, as shown in Fig. 5(b), the highest superconducting transition temperature is about 40 K due to the relatively small $c$-axis lattice constants.

V. HOW TO ACHIEVE A HIGHER $T_c$ IN THE IRON-BASED SUPERCONDUCTORS?

By adjusting the sample carrier concentration and improving the sample quality, it may still be possible to raise the $T_c$ of the iron-based family by a few more kelvins. According to our theory, increasing the $c$-axis lattice constant appeared to be the most effective method of enhancing $T_c$ in FeAs family. In what follows, we will estimate roughly the $c$-axis lattice constant values that can make the $T_c$ of iron-based materials into the liquid nitrogen range (77 K), and even 100 K.

According to the lattice constants, we now have two classes of the iron-based superconductors: the $c/a \approx 3$ class and the $c/a \approx 5/2$ class. From the experimental data of Table I and Table II, we can obtain two characteristic parameters for each class. They are $T_c^{max}(1) = 55$ K and $c_1 = 8.428\,\AA$ for the $c/a \approx 3$ class and $T_c^{max}(2) = 38$ K and $c_2 = 6.606\,\AA$ for the $c/a \approx 5/2$ class. By applying the hypothesis of Eq. (6), we have

$$E[T_c(1), c_1] = E[T_c(2), c_2],$$

$$\alpha_1 T_c^{max}(1) + \beta_1 \frac{1}{c_1} = \alpha_2 T_c^{max}(2) + \beta_2 \frac{1}{c_2},$$

(7)
FIG. 8: The relationship between $T_c$ and the $c$-axis lattice constants based on the reported experimental data. (a) For the large $c$ iron-based superconductors, and (b) for the short $c$ iron-based superconductors. Our predictions of the maximum $T_c$ for both classes are also shown in the figures.

where $(\alpha_1, \beta_1)$ and $(\alpha_2, \beta_2)$ are material-related parameters.

For ease of discussion, we further assume $\alpha_1 = \alpha_2 = \alpha_I$ and $\beta_1 = \beta_2 = \beta_I$, then we can redefine a unified parameter by the using of Eq. (7)

$$\lambda_I = \frac{\beta_I}{\alpha_I} = \frac{c_1c_2}{c_2 - c_1} \Delta T_c^{\max}$$

$$(8)$$

By applying the experimental data, one can obtain

$$\lambda_I = \frac{8.428 \times 6.606 \times (55 - 38)}{(8.428 - 6.606)} = 519.5.$$ 

We consider that the estimated value of $\lambda_I = 519.5$ is the general characteristic parameter of the iron-based superconductors. This parameter may help point the way to finding variants of the FeAs materials with higher $T_c$. Eq. (8) can be rewritten as

$$c_2 = \frac{\lambda_I \times c_1}{\lambda_I - (T_c^{\max(2)} - T_c^{\max(1)}) \times c_1}.$$ 

From the above equation, we now have three known parameters: $c_1 = 8.428 \, \text{Å}$, $T_c^{\max(1)} = 55 \, \text{K}$ and $\lambda_I = 519.5$. For a given target superconducting transition temperature $T_c^{\max(2)}$, it is very easy to get the corresponding $c$-axis lattice constant $c_2$. Figure 9 shows the results for two target temperatures: $T_c^{\max(2)} = 77 \, \text{K}$ and $100 \, \text{K}$. These results indicate that in order to raise $T_c$ into the liquid nitrogen range (77 K), the $c$-axis lattice constant should at least reach $13 \, \text{Å}$. For even higher $T_c$, for example $T_c = 100 \, \text{K}$, the $c$-axis lattice constant is estimated to be around $31.287 \, \text{Å}$. But in any case, the maximum superconducting transition temperature ($T_c^{\max}$) of the iron-based superconductors would not exceed 116.7 K, as indicated in Fig. 9.

VI. THE LATEST EXPERIMENTAL AND THEORETICAL RESULTS

Recently, the new type of Fe superconductor with a $T_c$ of approximately 8 K has been discovered for tetragonal FeSe compound [36]. Later the $T_c$ of 27 K for the FeSe superconductor at 1.48 GPa, showing an extremely high pressure coefficient of 9.1 K/GPa, has been reported [37]. The crystal structure of the FeSe is the simplest among the reported iron-based superconductors with the
FIG. 10: The lager $c$-axis unit cell discovered in (a) the LaO$_{1-x}$F$_x$FeAs superconductor, and (b) the (Sr$_3$Sc$_2$O$_5$)Fe$_2$As$_2$ parent compound for the FeAs-based superconductors.

shortest $c$-axis lattice constant $c \approx 5.52\text{Å}[37]$ and the smallest value of $c/a \approx 2$, where $a = 3.7696/\sqrt{2}\text{Å}$. From our mechanism, the FeSe-related superconductors has the lowest $T_c^{\text{max}}$ due to a relatively shorter $c$-axis lattice constant. The corresponding $T_c^{\text{max}}(2)$ can be estimated by

$$T_c^{\text{max}}(2) = T_c^{\text{max}}(1) + \frac{\lambda_f \times (c_2 - c_1)}{c_1 \times c_2}.$$  

Roughly, we use $T_c^{\text{max}}(1) = 55\text{ K}$, $c_1 = 8.428\text{Å}$, $c_2 \approx 5.52\text{Å}$ and $\lambda_f = 519.5$ and obtain $T_c^{\text{max}}(2) \approx 24\text{ K}$, which is very close to the experiment value of 27 K[37]. Even taking into account all possible factors, we consider that the $T_c^{\text{max}}$ of the FeSe family is impossible to exceed $30\text{ K}$ because of the limitation of the short $c$-axis lattice constant.

We have been concerned about two interesting papers published on the ArXiv.org [38, 39]. In the LaO$_{1-x}$F$_x$FeAs Superconductor [38], Shekhar et al. found that apart from the standard phase ($c = 8.716\text{ Å}$) there exists another structural phase with a larger $c$-axis lattice constant of $c = 12.67\text{Å}$ ($c/a \approx 4.5$) as shown in Fig. 10 (a). If the authors can successfully synthesize some pure samples of $c = 12.67\text{Å}$ around the following doping levels $x = 1/8 = 0.125$, $2/15 \approx 0.133$, $2/9 \approx 0.222$ and $2/5 = 0.4$, we are confident that their $T_c$ can easily break through 60 K, perhaps reach about $T_c = 70\text{ K}$. At the same time, Zhu et al. fabricated a possible new parent compound for the FeAs-based superconductors[39], namely (Sr$_3$Sc$_2$O$_5$)Fe$_2$As$_2$ with the lattice constants $a = 2.876\text{Å}(4.0678/\sqrt{2})$ and $c = 13.424\text{Å}(26.8473/2)$ ($c/a \approx 4.67$), as shown in Fig. 10 (b). Based on the new concept of superconductivity, we suggest the synthesis of some new related compounds (Re$_2$Sr$_{3-x}$Sc$_2$O$_5$)Fe$_2$As$_2$ (Re = La, Sm, Gd, Ce, Nd, ... ) at the following values of $x = 2/3 \approx 0.667, 2/5 = 0.4$ and $1/4 = 0.25$. The superconducting transition temperature of these samples is likely closed to or even exceed $T_c = 70\text{ K}$.

Interestingly, from a chemist’s viewpoint, Steele [40, 41] considered that the iron-based materials (PbO)$_x$FeAs, (BaO)$_x$FeAs and (BaO)$_x$FeP ($x = 1, 2$ or $3$) materials may also be the candidate of the higher $T_c$ superconductors.

VII. BRIEF SUMMARY

We have studied the maximum superconducting transition temperature ($T_c^{\text{max}}$) problems in the newly discovered iron-based superconductors. It has been shown clearly that all the reported FeAs superconductors can be divided into two basic classes depending on the lattice constants, they are the $c/a \approx 3$ class of the larger $c$-axis lattice constant and the $c/a \approx 5/2$ class of the shorter $c$-axis lattice constant. The results indicated that the former class has a maximum $T_c^{\text{max}} < 60\text{ K}$, while the latter class has a lower $T_c^{\text{max}} \leq 40\text{ K}$. In order to enhance $T_c^{\text{max}}$ in the iron-based superconductors, new class of FeAs compounds with a larger ratio of $c/a$ and $c$-axis lattice constant are suggested. We pointed out that their $T_c^{\text{max}}$ values could be raised into the liquid nitrogen range (77 K) and 100 K, supposing the new analogues with $c/a \approx 5$ (approximately $c \approx 13\text{ Å}$, if $a = 2.750\text{Å}$) and $c/a \approx 11$ ($c > 31\text{ Å}$) can be successfully synthesized in laboratory. Finally, the possible new ways to raise $T_c$ in the iron-based superconductor have been proposed based on the new experimental results.

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