Effects of isoelectronic Ru substitution at the Fe site on the energy gaps of optimally F-doped SmFeAsO

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Abstract

We studied the effects of isoelectronic Ru substitution at the Fe site on the energy gaps of optimally F-doped SmFeAsO by means of point-contact Andreev-reflection spectroscopy. The results show that the SmFe₁₋ₓRuxAsO₀.₈₅F₀.₁₅ system keeps a multigap character at least up to x = 0.50, and that the gap amplitudes Δ₁ and Δ₂ scale almost linearly with the local critical temperature Tc. The gap ratios 2Δ₁/kBTc remain approximately constant only as long as Tc ≥ 30 K, and increase dramatically when Tc decreases further. This trend seems to be common to many Fe-based superconductors, irrespective of their family. Based on first-principle calculations of the bandstructure and of the density of states projected on the different bands, we show that this trend, as well as the Tc dependence of the gaps and the reduction of Tc upon Ru doping, can be explained within an effective three-band Eliashberg model as being due to a suppression of the superfluid density at finite temperature that, in turn, modifies the temperature dependence of the characteristic spin-fluctuation energy.

(Some figures may appear in colour only in the online journal)

1. Introduction

The discovery of Fe-based superconductors (FeBSs) [1] with Tc as high as 55 K has shown that cuprates no longer represent the only class of high-Tc compounds. One of the reasons for the great excitement in the scientific community and for the impressive amount of work produced up to now is certainly that these materials give the opportunity to study high-Tc superconductivity in different systems, in the hope of identifying its key elements. The parent stoichiometric compounds of most FeBSs are not superconducting (with a few exceptions, like LiFeAs and LaFePO) but display a metallic behavior (as opposed to the Mott insulating state of cuprates) and feature a long-range antiferromagnetic (AFM) spin-density-wave (SDW) order. Superconductivity appears upon doping and, in some systems, also by applying pressure; however, the order of the transition between magnetic and superconducting phases seems not to be universal although increasing evidence is being collected of a region of coexistence of superconductivity and magnetism. In contrast to cuprates (where the superconducting region in the phase diagram is dome-shaped and the maximum Tc corresponds to a well-defined ‘optimal’ doping) in FeBSs superconductivity sometimes appears with Tc already very close to the maximum and shows a weak doping dependence in a broad doping range. A central feature of FeBSs—which is tightly connected to the origin of superconductivity according to the most widely accepted theories—is their multiband character. They feature indeed two or three hole pockets around the Γ point of the first Brillouin zone and two electron pockets at the M point.
In 1111 compounds, all the relevant Fermi surface sheets are weakly warped cylinders parallel to the $k_z$ axis (as expected in a layered material) while a greater degree of three-dimensionality is observed in 122 compounds. These multiple bands and their almost perfect nesting in the parent compound explain the AFM instability. The weakening of the nesting induced by doping instead leads to spin fluctuations that would act as the glue for the formation of Cooper pairs. A spin-fluctuation-mediated pairing would be mainly interband and would favor the opening of superconducting energy gaps of different signs on different Fermi surface sheets, the so-called $s\pm$ symmetry [4]. Although many theoretical and experimental results support this theory [5, 6] there is not, up to now, a definitive proof of such a picture. Things are further considerably complicated by the fact that the electronic bandstructure is very sensitive to some fine structural parameters, like the Fe–As–Fe bond angle and more particularly the height of the pnictogen atom ($h_{\text{As}}$) above the Fe layer. Possibly because of this sensitivity, in many situations the gap structure of FeBSs can vary considerably within the same system, giving rise to line nodes, point nodes, deep gap minima, etc [7–10].

In 1111 compounds, $h_{\text{As}}$ has been proposed as a switch between high-$T_c$ nodeless superconductivity and low-$T_c$ nodal superconductivity [11].

In an effort to discriminate the effects of different parameters on the superconducting and magnetic phases of FeBSs many different chemical substitutions have been performed. The main effect of aliovalent substitutions is to dope the parent compound with charge, either electrons [12, 13] or holes [14], thus allowing the phase diagram to be explored. Isovalent substitutions [15–18] instead have been tried to modify the lattice structure, create 'chemical pressure', introduce disorder (acting as magnetic or non-magnetic impurities), etc. A further degree of freedom is the site of substitution, that can reside either in the spacing layer [14] or in the active one containing Fe [15–18], which is possibly directly involved in the magnetic pairing via spin fluctuations.

Here we report on point-contact Andreev-reflection spectroscopy (PCARS) measurements performed in SmFe$_{1-x}$Ru$_x$AsO$_{0.85}$F$_{0.15}$ with $x$ ranging from 0 to 0.50. The considerable decrease of $T_c$ in this series of samples has been attributed to disorder in the Fe sub-lattice [15] and/or occurrence of a short-range static magnetic order [19]. The PCARS results clearly indicate the presence of a multigap character at all the investigated levels of Ru substitution. The superconducting gaps decrease approximately linearly with the local critical temperature of the contact, $T_{\Delta}^A$ but, even when the latter is reduced by a factor of 5 with respect to the optimal value, they show no sign of nodes, either intrinsic or ‘accidental’. For both gaps, the $2\Delta /k_B T_c$ ratio is rather constant down to $T_c^A \sim 30$ K but then increases consistently below this critical temperature. Comparison with other results in the literature indicates that many different FeBSs fit in this trend, which suggests the possibility of studying some properties common to different compounds in a single sample series that allows spanning of a very wide range of critical temperatures. Thanks to $ab$ initio electronic structure calculations, the trend of the gaps as a function of $T_{\Delta}^A$ has been reproduced within a minimal three-band, $s\pm$ Eliashberg model. This model also takes into account the so-called 'feedback' effect, i.e. the effect of the condensate on the antiferromagnetic spin fluctuations possibly responsible for the superconductivity in these compounds. The evolution as a function of $T_c$ of the temperature dependence of the condensate necessary to reproduce the experimental data looks rather similar to that obtained from London penetration depth measurements performed in other FeBSs, particularly in the region of coexistence of superconductivity and magnetism. This fact suggests that, in agreement with [19], the proximity of superconductivity and magnetism in these samples might be one of the main reasons for the decrease of $T_c$ and the observed behavior of the energy gaps.

2. Experimental details

The polycrystalline SmFe$_{1-x}$Ru$_x$AsO$_{0.85}$F$_{0.15}$ samples were synthesized as described in [15]. The starting mixture of a fine powder of SmAs and 99.9% pure Fe$_2$O$_3$, RuO$_2$, FeF$_2$, Fe and Ru was pressed into pellets and then put through a two-step reaction process involving a first heating to 450°C and a second heating to 1000–1075°C. X-ray diffraction analysis showed small amounts of SmOF (up to 6%) in the final samples. Figure 1 shows the dependence of the lattice constants $a$ and $c$ on the Ru content $x$, indicating that Ru substitution for Fe is effective. The resistive critical temperatures and residual resistivities for the samples used in this work are reported in table 1. The samples with $x = 0.25$ and 0.50 have higher $T_c$ and much improved transport properties (namely, resistivity, magnetoresistance and Hall mobility) than those reported in [15] for the same doping contents, even though they were prepared in the same way. The possible reason of this difference is under investigation. In any case, these samples were particularly suited for PCARS measurements, since the longer mean free path makes it easier to attain the spectroscopic conditions, as explained below.

Point-contact spectroscopy is a local, surface-sensitive technique and it is therefore necessary to avoid any surface
Figure 2. Temperature dependence of the raw conductance curve of a point contact on the $x = 0.10$ sample. The normal-state resistance is $R_N = 50 \, \Omega$. The inset shows the curves at 4.2 K and 21.0 K in an extended voltage range, to highlight the excess conductance persisting up to about 100 mV.

Table 1. Resistive critical temperatures and residual resistivities (defined as in [15]) for SmFe$_{1-x}$Ru$_x$AsO$_{0.85}$F$_{0.15}$ samples at different Ru contents. The $T_c$ and $\rho_0$ for the samples with $x = 0.25$ and 0.50 are different from those reported in [15].

| $x$  | $T_c$ (K) | $\rho_0$ (m$\Omega$ cm) |
|------|----------|--------------------------|
| 0    | 52.0     | 0.33                     |
| 0.05 | 42.8     | 0.87                     |
| 0.10 | 21.5     | 1.33                     |
| 0.25 | 28.1     | 1.20                     |
| 0.30 | 13.6     | 1.69                     |
| 0.50 | 13.5     | 0.70                     |

degradation or contamination. The samples were thus always kept in dry atmosphere, and broken to expose a clean surface prior to point-contact fabrication. The point contacts were made by putting a small drop of Ag paste on that surface, as described elsewhere [20, 21]. With respect to the standard ‘needle–anvil’ technique, this configuration ensures a greater mechanical and thermal stability of the contacts and also allows the whole mounting for point contact to be hermetically closed in the cold head of the cryogenic insert thus avoiding any exposition to air and moisture during the transfer from the glove box (where the point contacts are fabricated) to the cryogenic environment. Although the Ag drop has a diameter of at least 50 $\mu$m, the real electric contact occurs only between some of the Ag grains and the sample surface. The true contact is thus the parallel of several nanoscopic junctions that can well be in the ballistic regime (i.e. have radii smaller than the electron mean free path). In [15] a rough evaluation of the mean free path in SmFe$_{1-x}$Ru$_x$AsO$_{0.85}$F$_{0.15}$ gave $\ell \approx 3–10$ nm without any clear dependence on the Ru content. In the cleaner samples with $x = 0.25$ and $x = 0.50$, the same evaluation gives $\ell \approx 7$ nm and $\ell \approx 20$ nm, respectively. Such small values of the mean free path make the fulfilment of the ballistic condition $a \ll \ell$ (where $a$ is the contact radius) very difficult to achieve. For instance, with these values of $\ell$ and the residual resistivities taken from table 1, the Sharvin equation [22] would require resistances of the order of several $k\Omega$ for the contact to be ballistic. The typical experimental resistance of the contacts is instead in the range 10–100 $\Omega$. Indeed, many of the contacts were not spectroscopic or showed heating effects. A large number of measurements was then necessary to achieve a relatively small number of successful measurements. All the results reported here, except those shown in figure 3, are thus referred to the small fraction of contacts that do not show heating effects and give a clear Andreev-reflection signal. In these cases, the existence of many parallel nano-junctions can be invoked to reconcile the actual contact resistance with the requirement of ballistic transport [21]. In some cases, the Sharvin condition was fulfilled at low temperature but broke down on increasing the temperature because of the decrease in the mean free path. In these cases, the values of the gaps at low temperature can be taken as meaningful anyway, although their temperature dependence and eventually the value of the local critical temperature can be slightly affected by the non-ideality of the contact.

3. Results and discussion

3.1. Point-contact Andreev-reflection results

Figure 2 reports the temperature dependence of the raw conductance curves (obtained by numerical differentiation of the $I$–$V$ characteristics) of one of the contacts that did not
show any anomaly. The curves were measured in the $x = 0.10$ sample, and the normal-state resistance of the contact was around 50 $\Omega$. The curves show the typical features already observed in SmFeAs(O$_{1-x}$)F$_x$ [23], in LaFeAs(O$_{1-x}$F$_x$) [20] and in other 1111 compounds. In particular, they feature clear maxima related to a presumably nodeless gap, shoulders suggestive of a second larger gap and additional structures that, as recently shown [24], can be explained as being due to the strong electron–boson coupling. The excess conductance at high voltage, extending up to about 100 mV (see inset), is also typical of these systems [24]. The temperature at which the Andreev-reflection features disappear and the conductance becomes equal to the normal-state one is the local critical temperature of the contact, or Andreev critical temperature $T^A_c$. As shown in figure 2 this temperature is easy to identify in spectroscopic contacts because it also marks the point where conductance curves recorded at slightly different temperatures start to be superimposed on one another (here the curves at 21.0, 22.0 and 23.0 K coincide within the experimental noise).

In contrast, figure 3 reports two examples of conductance curves that show, together with an Andreev signal, deep and wide dips that, at low temperature, occur at energies comparable to those of the large gap. As shown elsewhere [21, 25], these dips are likely to be due to the current becoming overcritical in the region of the contact and prevent a proper determination of the gap amplitudes. On increasing the temperature, they move toward lower voltage (due to the decrease of the critical current), causing an apparent shrinkage of the Andreev signal, finally giving rise to a sharp cusp at zero bias.

Going back to the case of ballistic contacts as in figure 2, the conductance at or just above $T^A_c$ can be used to normalize all the curves at $T < T^A_c$. In principle, a conductance curve recorded at a given temperature should be normalized to the normal-state conductance at the same temperature, but because of the very high upper critical field of these materials, the latter is not usually accessible, at least at low $T$. Using the normal state at $T^N_c$ to normalize all the curves is thus a somehow arbitrary choice but, as shown elsewhere [24], is anyway the one that preserves the weaker structures, i.e. those due to the large gap and, if present, those due to the strong electron–boson coupling.

Figure 4 shows some examples of low-temperature, normalized conductance curves in samples with different Ru contents. Some important points are immediately clear by looking at these curves. First, none of them display zero-bias peaks, and the same happens in 100% of the spectroscopic contacts. These points toward the absence of line nodes even at the highest Ru contents, in contrast to what has been observed in some other FeBSs away from optimal doping [7–10]$.^6$ Second, all the curves show more or less marked double-gap features. Third, despite the very large range of doping, the widths of the structures do not change very much (note that all the panels have the same horizontal scale). Thus we should not expect major variations in the gap values upon Ru doping. Fourth, the asymmetry of the normalized conductance curves for positive/negative bias—which is particularly strong in unsubstituted SmFeAs(O$_{0.85}$F$_{0.15}$) [23]—seems to be reduced by Ru doping. As a matter of fact, it is clearly visible even at a first glance in the case $x = 0.05$, becomes discernible only while trying to fit the data in the cases $x = 0.10$ and 0.25 but almost completely disappears for $x = 0.30$ and 0.50. The real origin of this asymmetry, which is common to most point-contact spectra in Fe-based superconductors, remains not completely clear yet, though it has been recently ascribed to the Seebeck effect [28]. Preliminary Seebeck effect measurements performed in these samples show indeed a considerable decrease of the Seebeck coefficient with increasing Ru content [29].

Moreover, none of the curves we measured showed the finite-energy peaks associated with quasiparticle interference predicted, in some conditions, in the nodeless $\pm \pi$ symmetry [27]. The occurrence and the voltage positions of these peaks are controlled, in the relevant theory, by a mixing parameter $\alpha$ which has not been related yet to experimental parameters. Therefore, either these peaks are not present because the conditions for their observation are not fulfilled, or they are smeared out, particularly at the $Z$ values typical of our contacts, by the broadening effects.
The BTK model provides reliable results also in the case of parallel nano-junctions. Simulations show that the fit of the total conductance in the 2D case [26] and including a broadening term [31] is 1−1 (the weight of band 2 being consequently determined as w2=w1). The asymmetry decreases on increasing the Ru content, vanishing completely at x = 0.50. The fitting parameters are indicated in the labels.

To extract quantitative information about the amplitudes of the gaps from the conductance curves, they must be compared with suitable theoretical models. None of the models for single-band superconductivity can reproduce the shape of the experimental curves of figure 4. Instead, a two-band Blonder–Tinkham–Klapwijk model [30] generalized to the 2D case [26] and including a broadening term [31] is the minimal model that can be used in this case. For each band the parameters of the model are the energy gap Δ, the broadening parameter Γ and the barrier parameter Z. Then, as the total conductance is the weighed sum of the single-band conductances, the last parameter is the weight w1 of band 1 (the weight of band 2 being consequently determined as 1−w1). It is true that Sm-1111 is not really two-dimensional and thus a 3D model should be used; however, as shown elsewhere [24], the latter is much more complicated and for any practical purpose one can safely use the 2D model (especially when, as is the case here, the gaps are nodeless).

The lines in figure 4 represent the best fit of the experimental data, and the labels indicate the relevant values of the gaps and of the weight of band 1 in the point-contact conductance, w1. To account for the residual asymmetry of the normalized curves, we chose to fit the positive- and negative-bias sides separately (blue and red lines, respectively). As previously stated, for x ≥ 0.30 the asymmetry is very small and the difference between the two fits can no longer be appreciated.

Figure 5 shows two examples of how the normalized conductance curves evolve with temperature, and the resulting temperature dependence of the gaps extracted from the fit. The two cases shown refer to a lightly doped sample (x = 0.10) and to a heavily doped one (x = 0.50). The lowest-temperature curves show clear shoulders related to the larger gap, which become less and less discernible in the other curves (vertically offset for clarity). In the x = 0.50 case, a small dip structure is also seen to shift to lower energy on increasing the temperature, possibly giving rise to the small downward deviation of the temperature dependence of the large gap Δ2 from the BCS-like Δ(T) curve observed at high temperature. Although there is no reason to expect the gaps to follow a BCS-like curve, the effects of the dip do not allow us to discuss whether this deviation is intrinsic or is an artifact due to the small mean free path of the samples. Incidentally, on the basis of recent calculations within a minimal three-band Eliashberg model [32], one would instead expect the gaps to be greater than the BCS value in the proximity of the critical temperature.

Let us just recall here that the fitting procedure is generally not univocal, i.e. different sets of parameters can give almost equally good fits. The error bars in the insets to figure 5 indicate the spread of gap values resulting from different fits.

Figure 6(a) shows the behavior of the gaps as a function of the Ru doping x. The data are rather scattered but a general trend is anyway discernible. While the small gap Δ1 does not vary noticeably on increasing the Ru content x, the large gap Δ2 shows a rapid decrease from x = 0 to 0.10 and then remains approximately constant. This behavior is in rough qualitative agreement with that of the bulk Tc reported in table 1. Since PCARS is a local probe, the scattering of gap values at the same composition is most probably due to slight inhomogeneities in the local doping content. As long as Tc has a strong dependence on the doping content, i.e. up to x = 0.25, different point contacts on the same sample can thus provide different values of the gaps and of the local Tc, i.e. the Andreev critical temperature. As a matter of fact if one plots the gaps as a function of Tc as in figure 6(b), a roughly linear trend of both Δ1 and Δ2 can be appreciated despite the fluctuations in their values. It is worth recalling that the data reported here are already the results of a very careful selection aimed at eliminating all the questionable results, so that these fluctuations are not due to spurious effects that can be ascribed to non-ballistic conduction, heating, or spreading resistance. For the large gap,
Figure 5. Temperature dependence of the normalized conductance curves (symbols) of point contacts on the samples with $x = 0.10$ (a) and $x = 0.50$ (b) with the relevant two-band fit (lines). All the curves except the top ones are vertically shifted for clarity. The insets show the temperature dependences of the gaps $\Delta_1$ and $\Delta_2$ as extracted from the fit. The error bars indicate the spread of gap values obtained by different fits, when the other parameters ($\Gamma_i$, $Z_i$ and the weight $w_i$) are changed as well.

A large uncertainty was also found in the starting compound SmFeAs(O$_{1-x}$F$_x$) [23] (here represented by the vertical error bar on the point at the maximum $T_{c}^{d}$) and was ascribed to the residual degrees of freedom in the normalization process, to the asymmetry of the curves and to the fact that the features related to $\Delta_2$ are less sharp than those related to the small gap $\Delta_1$. However, in the high-doping range ($x = 0.3$ and 0.5), $T_{c}^{d}$ depends very little on the Ru content and the asymmetry has almost completely disappeared; even large differences in local composition correspond to small differences in $T_{c}^{d}$. Therefore, the spread of gap values accompanied by a small spread in $T_{c}^{d}$ seems to indicate a lack of correlation between these quantities (as observed also in MgB$_2$ with Al and Li co-doping [33]).

Since the gaps show an overall linear trend as a function of the local $T_{c}^{d}$, it is particularly instructive to plot the gap ratios $2\Delta_i/k_B T_c$ as a function of $T_{c}^{d}$. This is done in figure 7, which also reports various other PCARS data in 1111 and 122 compounds. Only results showing nodeless order parameters are shown for consistency. It is clear that the Ru substitution in the optimally F-doped Sm-1111 allows spanning of a wide range of critical temperatures, which not only covers but also
extends the range of $T_c$ values of superconducting Fe-based compounds measured so far by PCARS. As already shown in [24], the $2\Delta_1/k_B T_c$ ratios start to increase below $T_c \sim 30$ K. Surprisingly, PCARS data on this single sample series, namely SmFe$_{1-x}$Ru$_x$AsO$_{0.85}F_{0.15}$, feature basically the same behavior as those obtained from many other different nodeless FeBSs of the 1111 and 122 families.

These results appear to be in contrast to those reported in [34], where an opposite trend is suggested. However, even in the aforementioned paper, several results reported for FeBSs show $2\Delta_1/k_B T_c$ ratios which seem to increase with decreasing $T_c$, particularly for the large gap. A definitive answer on the possibility of a universal trend of $2\Delta_1/k_B T_c$ versus $T_c$ requires more experimental work, comparing results obtained with different techniques on samples of increasingly better quality.

3.2. Electronic structure calculations

In order to try to explain the observed PCARS data within the Eliashberg theory, we first performed electronic structure calculations. In particular, SmFeAsO electron and hole densities of states (DOSs) were obtained by *ab initio* calculations performed in the local density approximation to the density-functional theory (LDA-DFT) [35] as implemented in the all-electron full-potential APW and local orbitals [36, 37] code Wien2k [38]. APW has the advantage of treating explicitly Sm 4f electrons within the valence band yielding state-of-the-art band structure dispersion quality. To simulate Ru substitution our calculations were performed in a tetragonal super-cell containing four formula units ($Pma2_1$ No. 28) where 25% Ru concentration was achieved by the substitution of one Ru out of four Fe, retaining...
Figure 8. The SmRu$_3$Fe$_{1−x}$As fat-band structure in the four formula unit super-cell. The dots are proportional to the Fe 3d character of the wavefunctions. The parabolas show the results of a fit of the Fe 3d bands within the two-dimensional electron gas model. The upper and lower horizontal dashed lines are $E_F$ with and without F doping, respectively. (a) Reference band structure with La replacing Sm. (b) Actual SmOFeAs band structure including the 4f Sm bands. The two light hole bands have similar dispersions and have been fitted with a single parabola $h_1$. (c) The same as (b) but in the case of SmFe$_{0.75}$Ru$_{0.25}$AsO. In (b) and (c) the parabolic fit of band $e_3$ is shown only up to an energy close to the one where its hybridization with Sm 4f bands takes place.
for by the rigid shift of $E_F$ by 0.15 electrons per formula unit. Given the DOS $N(E)$ of the system, the shift can be simply estimated as $0.15/N(E_F)$. Anyway, care should be taken in defining $N(E)$, since the localized nature of the Sm 4f orbitals makes it likely that they do not receive the additional doping charge from F. We therefore filtered out this contribution from $N(E)$ considering only the contributions of the bands $e_{1,2}$ and $h_{1,2}$. Following this approach we obtained a sort of upper bound for the $E_F$ shift to be about 75 meV (90 meV) for SmFeAsO$_{0.85}$F$_{0.15}$ (SmFeO$_{0.75}$Ru$_{0.25}$AsO$_{0.85}$F$_{0.15}$). The Fermi levels $E_F$ of F-doped and undoped SmFeAsO and SmFeO$_{0.75}$Ru$_{0.25}$AsO are shown in figures 8(a)–(c). We see that in the F-doped systems the band $e_1$ is always partially filled, justifying our assumption of including its contribution in Eliashberg calculations. Regarding the effect of Ru substitution, by comparing figures 8(b) and (c) we see that the effect is modest; only band $e_2$ is a bit deeper and with a lower effective mass as shown in figure 8(c). The calculated DOSs and plasma frequencies for each band and for the two doping levels considered are reported in table 2.

### 3.3. Analysis of experimental results within Eliashberg theory

Based on the results of band structure calculations described so far, it is possible to propose an explanation of the experimental data by means of the simplest model that allows description of the essential physics of the materials under study. We used the three-band, $s$-wave Eliashberg theory [32] taking into account the feedback effect [41]. Within this model we have two hole bands (from now on labeled as 1 and 2) and one equivalent electron band (labeled as 3). The free parameters are $N_f(0)$, $\lambda_{31}$, $\lambda_{32}$, $\Omega(T)$ and $\Gamma$. $N_f(0)$ is the DOS at the Fermi level, calculated above for $x = 0$ and $x = 0.25$ and obtained at all the other doping levels by linear interpolation as a function of the experimental $T_c$; $\lambda_{31}$ and $\lambda_{32}$ are the electron–boson coupling constants between band 3 and band 1 or 2, respectively; $\Omega(T)$ is the representative boson energy that we take as $\Omega(T) = \Omega_0 \tanh(1.76k_\text{B}T_c/\hbar(T_c - T))$ where $\Omega_0 = 2T_c/\hbar$ [42]; the electron–boson spectral function has a Lorentzian shape [32] with halfwidth $\Gamma = \Omega_0/2$ [6]; $T_\ast$ is the feedback critical temperature, determined by solving the Eliashberg equations in the imaginary-axis formulation. The electron–boson coupling matrix is

$$
\begin{pmatrix}
0 & 0 & \lambda_{31}v_1 \\
0 & 0 & \lambda_{32}v_1 \\
\lambda_{31} & \lambda_{32} & 0
\end{pmatrix}
$$

where $v_1 = N_1(0)/N_f(0)$ and $v_2 = N_2(0)/N_f(0)$. $k$ was determined at $x = 0$ in the following way. First, the superfluid density was calculated by using the plasma frequencies obtained from first principles and reported in table 2, giving also the correct $T_c$. Then, since the temperature-dependent part of the superfluid density corresponds to that of the representative boson frequency [41], this curve was fitted with $\tanh(1.76k_\text{B}/(T_\ast(T_c - T)))$, giving $k = 0.6192$. The values of the calculated superfluid density and the relevant fit are shown in figure 9 as symbols and a line, respectively.

At this point, the only parameters that remain to be determined are $\lambda_{31}$ and $\lambda_{32}$. At $x = 0$ they are obtained by reproducing the two experimental gaps, but it turns out that they also reproduce the exact experimental critical temperature. Then we assume that the ratio $\lambda_{31}/\lambda_{32}$ is doping-independent and that $k$ is a linear function of the experimental critical temperature: $k(T_c) = k(T_c=x=0)T_c/T_c=x=0$. This assumption is related to the temperature dependence of the superfluid density and it is reasonable to suppose that with increasing $x$ (and therefore decreasing $T_c$) it decreases [8]. Now, the only free parameter left in the process of fitting the $T_c$ dependence of the gaps is $\lambda_{31}$ which is fixed by obtaining $T_c$ coincident with the experimental one. The procedure is self-consistent since $\lambda_{31}$ is varied until $T_c^\ast$, introduced in the formula for $\Omega(T)$, allows reproduction of the experimental $T_c$. Disorder effects have been neglected as impurities are dominant in the intraband channel and are thus not pair-breaking. Moreover, we also assumed that, as a first approximation, they are also absent in the interband channel since the two gaps are well distinct at all doping levels.

The results are shown in figure 6(b) as solid lines; the calculated gap values follow rather well the trend of the experimental ones at all temperatures. The same good agreement with the experiment can be seen also by looking at the $2\Delta_c/\hbar k_\text{B} T_c$ ratios as a function of $T_c$ shown in figure 7 which also reports many other results from the literature. In this regard, it is also remarkable that it is possible, with a relatively simple model and a small number of free parameters, to reproduce the increase of the ratio with decreasing $T_c$. Since the strength of the coupling increases with decreasing $T_c$, so does, as expected, the total electron–boson coupling constant, $\lambda_{\text{tot}}$, which is about 3.2 at $T_c = 52$ K and goes up to almost 7.3 when $T_c = 10$ K. Another interesting result that comes out from the theoretical analysis is the temperature dependence of the representative boson frequency (shown in the inset to figure 9 for different critical temperatures) which, as already stated above, is equivalent to that of the superfluid density [41]. We can notice that, as $T_c$ decreases, the superfluid density also decreases as a function of $T$ assuming, below $T_c = 30$ K, a positive curvature at intermediate temperatures. Similar dependences (at least in the low- and mid-$T_c$ range) have been obtained in penetration.
depth measurements in Co-doped Ba-122 samples, as reported in [8]. In that case the effect is less pronounced probably because the results are reported only down to about 2$T_{c,\text{opt}}$/5, where $T_{c,\text{opt}}$ is the critical temperature at optimal doping. In our case instead $T_c$ drops to $T_{c,\text{opt}}$/5 at the highest Ru doping. Moreover, it is also interesting to notice that in Co-doped Ba-122 the temperature dependence of the superfluid density looks slightly more depressed in samples that belong to the region of coexistence of superconductivity and magnetism. This fact leads us to speculate that the observed behavior of the superfluid density in our samples might be considerably influenced by the onset of a short-range magnetic order which competes with superconductivity and that has been observed by μSR and $^{75}$As NQR measurements in the same samples [19]. Penetration depth measurements, like the ones in [8], would help in clarifying this point as well as the experimental determination of the temperature dependence of the representative boson frequency, as carried out in [6, 24, 43].

4. Conclusions

The isoelectronic substitution of Fe with Ru in optimally F-doped Sm-1111 is a good way to explore a very wide range of critical temperatures within the same Fe-based compound, in principle without changing the total charge of the system [15]. The considerable decrease of $T_c$ induced by Ru substitution has been ascribed to disorder in the Fe sub-lattice [15] and/or to the onset of a short-range magnetic order [19]. Here we have shown that, in a wide range of $T_c$ (from 52 K down to 13.5 K, corresponding to Ru contents ranging from 0 to 50%), the Sm(Fe$_{1-x}$Ru$_x$)$_2$As$_2$O$_{5.5}$F$_{0.15}$ system retains its original multigap character, and also the symmetry of the gaps remains nodeless. The amplitudes of the two experimentally detectable gaps, $\Delta_1$ and $\Delta_2$, decrease almost linearly with $T_c$, but they remain well distinct down to the lowest $T_c$. This suggests that the substitution-induced disorder mainly enhances the intraband scattering and does not significantly affect the interband scattering. The gap ratios $2\Delta_i/k_B T_c$ strongly increase for $T_c < 30$ K in a manner which suggests an unexpected increase of the electron–boson coupling when $T_c$ is depressed. Very interestingly, the trend of the gap ratios as a function of $T_c$ in this single system is superimposed on the analogous trend obtained by plotting the data of many Fe-based compounds of different families [24]. Needless to say, this seems to point toward a general, universal property of this class of superconductors. By using the values of the densities of states and plasma frequencies calculated from first principles, we have shown that the increase in the gap ratios $2\Delta_i/k_B T_c$ on decreasing $T_c$ can be reconciled with a spin-fluctuation-mediated pairing even though the characteristic spin-fluctuation energy has been observed to decrease linearly with $T_c$. The key to solving this puzzle is the feedback effect, i.e. the effect of the condensate on the mediating boson, which is of course only expected when the superconducting pairing between electrons is mediated by electronic excitations [41]. An analysis carried out within an effective three-band Eliashberg model shows indeed that the experimental dependence of the gaps (and of the gap ratios $2\Delta_i/k_B T_c$) on $T_c$ can be explained as being due, in particular, to a change in the shape of the temperature dependence of the characteristic boson energy, $\Omega_0(T)$, with respect to the optimal-$T_c$ compound (with no Ru). Indeed, a suppression of $\Omega_0$ in the mid-temperature range (which becomes more and more noticeable on decreasing $T_c$) is required to obtain the correct critical temperature and the
correct gap values. This finding is in very good qualitative agreement with the experimental observation of a decrease of the superfluid density in Co-doped Ba-122 with reduced $T_c$ [8]. The fact that in the latter case this reduction is observed in underdoped samples that fall in the region of coexistence of magnetism and superconductivity further suggests that, also in our samples, the reduction of the superfluid density and the consequent decrease in the boson energy that occur at finite temperature may be considerably influenced by the onset of a short-range magnetic order competing with superconductivity induced by Ru substitution, as recently observed by $\mu$SR and $^{75}$As NQR measurements in the same set of samples [19].

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