Comment on “Isoelectronic Ru substitution at Fe-site in Sm(Fe$_{1-x}$Ru$_x$)AsO$_{0.85}$F$_{0.15}$ compound and its effects on structural, superconducting and normal state properties”
(arXiv:1004.1978)

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Based on the five-orbital model, we derive the reduced impurity scattering rate $g = g_{\text{imp}}/2\pi T_c$ in Sm(Fe$_{1-x}$Ru$_x$)AsO$_{0.85}$F$_{0.15}$ from the residual resistivity. At $x = 0$, the transition temperature is $T_c = 42 K$. For $0.05 \leq x \leq 0.36$ the obtained value of $g$ ranges from 1.5 to 2.9, which suggests that the s$_\pm$-wave state cannot survive. We point out that the magnetoresistance frequently gives an underestimated value of $g$ in correlated electron systems.

In Ref. [1], it was shown that the transition temperature in polycrystal Sm(Fe$_{1-x}$Ru$_x$)AsO$_{0.85}$F$_{0.15}$ at $x = 0$, $T_c = 50$ K, decreases to $T_c = 15$ K at $x = 0.36$, and $T_c = 0$ K at $x = 0.75$. The observed weak x-dependence of $T_c$ is consistent with previous reports [2, 3]. The authors discussed the reduced scattering rate $g = z\gamma/2\pi T_c$ where $\gamma$ is the electron scattering rate and $z = m/m^*$ is the renormalization factor. Theoretically, the sign reversal of the s-wave (s$_\pm$-wave) state vanishes for $g > g_{\text{imp}} = 0.23$ [4]; $g_{\text{imp}} < 1$ due to large interband impurity scattering, where all bands are composed of the same d-orbitals. Thus, it is essential to derive $g$ from experiments.

Here, we derive a reliable value of $g$ from the residual resistivity $\rho_0$, since we can calculate $\rho_0$ with enough accuracy due to the fact that the realistic five-orbital model is available [5]. In the linear-response theory, $\sigma_{xx} = \frac{e^2}{4\pi^2} \sum_i \int_{FS} dS_k |v_k| v_k^i \frac{|\nu_k^i|}{2\pi}$ [4], where $i$ represents the Fermi surfaces, $v_k^i = \nabla_k E_k^i$, and $c$ is the inter-layer spacing. Using the five-orbital model, we obtain the relation $\sigma_{xx}[\mu\Omega cm] = 0.24\gamma[K]$ in 1111 systems ($c = 0.8$nm) for the filling $n = 5.8 - 6.1$. Then, $g$ is given as $g = 0.66z \rho_0 / \rho_{\text{imp}}|T_c|$. In the derivation, correct physical quantities, such as carrier density and Fermi velocity, are maintained automatically. In the single crystal NdFeAsO$_{0.7}$F$_{0.3}$ with $T_c = 46.4$ K, $T_c$ decreases to $T_c/2$ by $\alpha$-particle irradiation when $\rho_0 \sim 480 \mu\Omega cm$. Thus, $T_c$ is halved when $g = 3.4 = 15 g_{\text{imp}}$ for $z = 1/2$.

Next, we discuss Sm(Fe$_{1-x}$Ru$_x$)AsO$_{0.85}$F$_{0.15}$. According to Fig. 15 of Ref. [1], $\rho_{\text{imp}} \sim 900 \mu\Omega cm$ at $x = 0.05$ ($T_c = 42$ K), which corresponds to $\rho_0 \sim 220 \mu\Omega cm$ in the single crystal, if we apply the empirical relation $\rho_{\text{imp}} / \rho_{\text{single}} \sim 4$ [2]. Since the corresponding $g$ is 1.5 for $z = 1/2$, s$_\pm$-wave state cannot survive against 5% Ru impurities, unless $\rho_{\text{imp}} / \rho_{\text{single}} > 26$. These results are consistent with the previous report for Nd1111 [2]. We also obtain $g \sim 2.9$ at $x = 0.36$ ($T_c = 15$ K) where $\rho_0 \sim 1750 \mu\Omega cm$. However, the reduced scattering rates derived from the magnetoresistance $\Delta \rho / \rho_0 \equiv (\mu_{\text{MR}} B)^2$ and Hall angle $\sigma_{xy}/\sigma_{xx} \equiv \mu_{\text{H}} B$ at $x = 0.36$ in Ref. [1] are $\mu_{\text{MR}} \sim 0.5$ and $\mu_{\text{H}} \sim 7.5$ at 57K, respectively [6]. For $0.05 \leq x \leq 0.33$, $g_{\text{MR}} = 0.9 - 1.5$ and $g_{\text{H}} = 1.1 - 7.5$ according to Fig. 12 of Ref. [1]. Thus, both $g_{\text{MR}}$ and $g_{\text{H}}$ exceed $g_{\text{imp}}$ for $x \geq 0.05$.

It should be noticed that $\mu_{\text{H,MR}}$ can prominently deviate from the true mobility in correlated metals. For example, the ratio $r \equiv \mu_{\text{MR}} / \mu_{\text{H}}$ is not unity in general. The inset of Fig. 3(b) in Ref. [1] shows that the relation $\Delta \rho / \rho_0 / (\sigma_{xy}/\sigma_{xx})^2 \equiv r^2 \sim 9$ holds in single crystal BaFe$_2$(As,P)$_2$, suggesting that $r \sim 3$. In high-$T_c$ cuprates, $r^2 \sim 3$ in Y- and Bi-based compounds, whereas $r^2 \approx 14$ in La$_{1-x}$Sr$_x$CuO$_4$ at $x = 0.17$ [8], and $r^2 \sim 100$ at $x \geq 0.23$ [9]. Thus, the material dependence of $r = \mu_{\text{MR}} / \mu_{\text{H}}$ is very large even in systems with single Fermi surface [11]. [For example, $r$ becomes large when mean-free-path is anisotropic[10].] Moreover, $\mu_{\text{H,MR}}$ can deviate from the true mobility below $\sim 200$ K due to the current vertex correction (CVC) in the presence of strong spin (or orbital) fluctuations [11]. In fact, Ref. [7] revealed the significant role of the CVC in BaFe$_2$(As,P)$_2$.

To summarize, we derived the expression $g = 0.66z \rho_0 \sim 15 \mu\Omega cm |T_c|$, which is reliable since $\rho_0 / \gamma$ essentially depends only on the averaged $k_F$ and $v_F$ for each Fermi surface, whereas insensitive to the correlation effects. For the s$_\pm$-wave state, the critical residual resistivity for $g_{\text{imp}} = 0.23$ is only 35 $\mu\Omega cm$ if $z \sim 1/2$. This fact supports the s$_\pm$-wave state predicted by the orbital-fluctuation theory [12]. Slow decrease in $T_c$ ($-\Delta T_c \sim 2K$ per 1% impurities) might originate from the localization effect or reduction of orbital fluctuations by impurities. In contrast to $\rho_0$, Hall angle and $\Delta \rho / \rho_0$ are not simply scaled by $g$ since they are sensitive to other factors, like the Fermi velocity anisotropy and the CVC. Therefore, we have to take care in deriving $g$ from them.

[1] M. Tropeano et al., arXiv:1004.1978; We are grateful to M. Tropeano for useful discussions.

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$T = 200 \text{ K}$, at which the CVC would be small.

[3] C. Tarantini et al., Phys. Rev. Lett. 104, 087002 (2010).

[4] S. Onari and H. Kontani, Phys. Rev. Lett. 103 177001 (2009); Theoretically, $\Delta \rho_0 \sim 20 \mu \Omega \text{cm}$ per 1% impurities with strong scattering potential ($I = 1 \text{ eV}$), which is consistent with Fe-site substitutions in Refs. [1, 2]. We find that $\gamma_i$ is approximately band-independent in the $T$-matrix approximation.

[5] K. Kuroki et al., Phys. Rev. Lett. 101, 087004 (2008).

[6] $g_{\text{poly}} = 30$ given by $\mu_\parallel \propto R_\text{H}/\rho$ in Ref. [1] corresponds to $g_{\text{single}} = 30/4 = 7.5$ in the single crystal.

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[8] J. M. Harris et al., Phys. Rev. Lett. 75, 1391 (1995).

[9] F.F. Balakirev et al., Phys. Rev. B 57, R8083 (1998).

[10] In the linear response theory, $\sigma_{xy}$ and the magneto-conductivity are respectively given by $\sigma_{xy} \sim B \sum_i (\langle |l_k|^2 (\partial \theta_k/\partial k_i) \rangle_{FS_i}$ and $\Delta \sigma_{xx} \sim -B^2 \sum_i (\langle |l_k|^2 (\partial \theta_k/\partial k_i)^2 \gamma_k^{-1} \rangle_{FS_i} + (\partial |l_k|/\partial k_i)^2 \gamma_k^{-1} \rangle_{FS_i}$, where $l_k$ is the mean-free-path including the CVC, and $\theta_k = \tan^{-1}(l_{kz}/l_{ky})$. Note that $\Delta \rho/\rho_0 = -\Delta \sigma_{xx}/\sigma_{xx} - (\sigma_{xy}/\sigma_{xx})^2$. Since the CVC enlarge $\partial \theta_k/\partial k_i$ near the cold-spot, both $R_\parallel$ and $\Delta \rho/\rho_0$ are enhanced near quantum-critical-points. In addition, $\Delta \rho/\rho_0$ becomes large when $l_k$ is anisotropic due to the second term in $\Delta \sigma_{xx}$.

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