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Annealing effect on the crystal structure and electronic property of $SrFe_2(As_{0.65}P_{0.35})_2$

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1 Introduction

It was found that post-annealing of as-grown crystals sometimes gives a remarkable change in the electronic properties of Fe-based superconductor (FeSC). For example, the large anisotropy in low-temperature in-plane resistivity of $BaFe_2As_2$ disappeared after annealing[1]. It suggests some intrinsic change in the electronic state with annealing treatment. Recently, we found that T_C is substantially enhanced by post-annealing in $SrFe_2(As,P)_2$ (P-Sr122). Since the electronic properties including superconductivity are quite sensitive to a small structural change in FeSC, we performed the x-ray diffraction analysis for as-grown and annealed $SrFe_2(As_{0.65}P_{0.35})_2$ single crystals to clarify the annealing effects on the crystal structure and electronic property.

2 Experiment

High-quality single crystals of $SrFe_2(As_{0.65}P_{0.35})_2$ (T_C = 26K for the as grown crystal and T_C = 33K for the annealed one) were grown using the self-flux method. The x-ray diffraction experiment for single crystals was carried out using the x ray with 15 keV at BL-8A of the Photon Factory. The data was refined by the least-squares method using Rigaku CRYSTALSTRUCTURE.

3 Results and Discussion

Table I shows the annealing effect on the crystal structure. The structure analysis clearly demonstrates that the annealed crystal has the shorter *a*-axis and longer *c*-axis than the as-grown crystal. In addition, the *z* position of As/P also increases, leading to a higher pnictogen height h_{Pn} and a smaller As-Fe-As bond angle. In FeSC, it has been pointed out that T_C is correlated with the pnictogen height and/or the As-Fe-As bond angle[2, 3]. Considering that T_C sharply changes around h_{Pn}~1.33 Å[2], a tiny extension of h_{Pn} in $SrFe_2(As_{0.65}P_{0.35})_2$ (~1.32 Å) can result in an enhancement of T_C.

Another important effect of post-annealing is to decrease disorders within the crystals. The reduction of disorders made the system cleaner and modified the gap feature as observed by the penetration depth and specific heat measurement[4, 5].

In conclusion, we performed the x-ray diffraction measurement to investigate the annealing effect on the crystal structure and electronic property. We found that T_C enhancement was caused by both the elongation of the pnictogen height h_{Pn} and the reduction of carrier scattering.

Compound	As grown	Annealed
Space group	$I4/mmm$	$I4/mmm$
a (Å)	3.8983(14)	3.8963(6)
c (Å)	12.064(4)	12.092(2)
V (Å^3)	183.33(11)	183.57(5)
Sr	(0, 0, 0)	(0, 0, 0)
Fe	(1/2, 0, 1/4)	(1/2, 0, 1/4)
As/P	(0, 0, z)	(0, 0, z)
	z = 0.359 31(6)	z = 0.359 56(5)
h_{Pn} (Å)	1.319(1)	1.325(1)
Bond lengths and angles		
Sr-As (Å)	3.2372(7)	3.2364(3)
Sr-Fe (Å)	3.5910(9)	3.5964(4)
Fe-As/P (Å)	2.3533(4)	2.3559(3)
Fe-Fe (Å)	2.7565(7)	2.7551(3)
As-Fe-As (deg.)	108.301(10) × 4	108.434(8) × 4
	111.84(2) × 2	111.566(17) × 2
Number of reflections [$I > 2.00\sigma(I)$]	211	219
Goodness of fit	3.315	6.018

Table. 1: Refined lattice constants, atomic positions, and bond lengths and angles at room temperature for the as-grown and annealed single crystals from the least-squares refinement of the single crystal x-ray diffraction profile. h_{Pn} was calculated from h_{Pn} = (z −0.25) × c. The reliabilities are $R_1[I > 2.00\sigma(I)]$ = 6.61%, 5.16% and $wR_2[I > 2.00\sigma(I)]$ = 10.17%, 8.15% for the as-grown and annealed crystals, respectively. The number of reflections is the number of diffraction peaks used for analysis.

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