Magnetic structure of EuFe$_2$As$_2$ determined by single crystal neutron diffraction

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Among various parent compounds of iron pnictide superconductors, EuFe$_2$As$_2$ stands out due to the presence of both spin density wave of Fe and antiferromagnetic ordering (AFM) of the localized Eu$^{2+}$ moment. Single crystal neutron diffraction studies have been carried out to determine the magnetic structure of this compound and to investigate the coupling of two magnetic sublattices. Long range AFM ordering of Fe and Eu spins was observed below 190 K and 19 K, respectively. The ordering of Fe$^{2+}$ moments is associated with the wave vector $\mathbf{k} = (1,0,1)$ and it takes place at the same temperature as the tetragonal to orthorhombic structural phase transition, which indicates the strong coupling between structural and magnetic components. The ordering of Eu moment is associated with the wave vector $\mathbf{k} = (0,0,1)$. While both Fe and Eu spins are aligned along the long $a$ axis as experimentally determined, our studies suggest a weak coupling between the Fe and Eu magnetism.

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I. INTRODUCTION

The recent discovery of pnictide superconductors has drawn extensive attention because it provides a new opportunity to investigate the mechanism of superconductivity [1, 2, 3, 4, 5]. Most of the research on pnictide superconductors has focused on RFeAs(O,F$_{1-x}$) (with $R =$ La, Nd and Sm) and AFe$_2$As$_2$ (with $A =$ Ba, Ca and Sr), the so-called ‘1111’ and ‘112’ families. These two families are closely related since both of them adopt a layered structure with a single FeAs layer in the unit cell of ‘1111’ and two such layers in the unit cell of ‘122’. The superconducting state can be achieved either by electron or hole doping of the parent compounds [6, 7]. Till now, the highest $T_c$ attained is 57.4 K in the electron doped Ca$_{0.4}$Na$_{0.6}$FeAsF ‘1111’ compound [10], while for ‘122’ family the highest $T_c$ of 38 K is reached in the hole doped Ba$_{0.4}$K$_{0.6}$Fe$_2$As$_2$ [9]. Considering that the electronic states near the Fermi surface are dominated by contributions from Fe and As, it is believed that the FeAs layers are responsible for superconductivity in these compounds.

Recent neutron diffraction experiments reveal that the formation of the spin density wave (SDW), originating from the long range antiferromagnetic (AFM) order of the Fe moments at low temperature, seems to be a common feature for all the iron pnictide parent compounds [11, 12, 13, 14, 15]. The onset of the AFM order is also accompanied by the Tetragonal-Orthorhombic (T-O) structural phase transition in the ‘122’ family and preceded by the T-O phase transition for the ‘1111’ family. Phase diagrams of some iron pnictides clearly show that the magnetic order is suppressed with appropriate charge carrier doping of parent compound. Concomitantly, superconductivity emerges and reaches a high $T_c$ at optimal doping [16], thus exhibiting features similar to high $T_c$ cuprates [17]. It is generally believed that the superconductivity in iron pnictides is unlikely due to simple electron-phonon coupling, as demonstrated from extensive studies of phonon dynamics [18, 19]. Magnetism seems to play a crucial role in the appearance of superconductivity and AFM spin fluctuations have thus been suggested to be a possible paring mechanism. Strong evidence on the presence of resonant spin excitation in the superconducting phase has indeed been obtained from recent inelastic neutron scattering experiments on several optimally doped ‘122’ superconductors [20, 21, 22, 23].

EuFe$_2$As$_2$ is a peculiar member of iron arsenide AFe$_2$As$_2$ family since the A site is occupied by Eu$^{2+}$, which is an S-state (orbital angular momentum $L = 0$) rare-earth ion possessing a 4f$^7$ structure with the electron spin $S = 7/2$. The theoretical effective magnetic moment of Eu$^{2+}$ ion is 7.94 $\mu_B$. As revealed by Mössbauer and magnetic susceptibility measurements on single crystals, the Eu$^{2+}$ moments order antiferromagnetically below $T_N \sim 20$ K [24, 25]. It is also reported that the moment of Eu$^{2+}$ can be realigned ferromagnetically by applying a magnetic field [26, 27]. Besides, superconductivity can also be achieved by replacing Eu by alkali metals, e.g. the $T_c$ is observed to be 31 K and 34.7 K for Eu$_{0.8}$K$_{0.2}$Fe$_2$As$_2$ [28] and Eu$_{0.3}$Na$_{0.7}$Fe$_2$As$_2$ [29], respectively. Unlike BaFe$_2$As$_2$, in which the superconductivity emerges with the Ni substitution of Fe, the SDW is suppressed in EuFe$_{2-x}$Ni$_x$As$_2$ without the emergence of superconductivity [30]. Furthermore, the magnetic ordering of Eu$^{2+}$ moments evolves from AFM to ferromagnetic at higher levels of Ni doping.

Since magnetism and superconductivity appears to be in-
mately related in iron pnictides, it is therefore equally importance to understand the magnetic properties especially for the compounds that contain the magnetic lanthanide ions. The investigation of the interplay between the lanthanide and iron magnetism may also be crucial for a deeper understanding of the magnetic and electronic properties of iron pnictides. For EuFe$_2$As$_2$, the magnetic ordering and the details of magnetic structure have not been clarified so far via single-crystal neutron diffraction due to the extremely large neutron absorption cross-section of Eu. Here we report neutron diffraction studies on a high-quality EuFe$_2$As$_2$ single crystal using the hot neutron source. It has been observed that both the Fe$^{2+}$ and Eu$^{2+}$ moments are ordered antiferromagnetically below 190 K and 19 K, respectively. A unique propagation vector $k = (1,0,1)$ is determined for the Fe magnetic sublattice with the K and 19 K, respectively. A unique propagation vector aligned along the a axis. Furthermore, the magnetic propagation vector is determined to be $k = (0,0,1)$ for the Eu$^{2+}$ moment, which is also aligned along the a axis. The coupling between the Fe and Eu magnetic sublattices has been found to be rather weak. The determination of the magnetic structure of EuFe$_2$As$_2$ would pave the way for further investigations of EuFe$_2$As$_2$ under high pressure and strong magnetic fields.

II. EXPERIMENT

EuFe$_2$As$_2$ single crystals were grown by the flux method. A small amount of powdered single crystal was examined by means of x-ray powder diffraction (XRD) analysis. The XRD pattern reveals a single phase of EuFe$_2$As$_2$ in the tetragonal ThCr$_2$Si$_2$ structure with space group $I4/mmm$ at room temperature. The samples have also been characterized via the measurements of heat capacity, resistivity and magnetic susceptibility. Two prominent phase transitions can be identified respectively at 190 and 19 K, consistent to those previously reported [24, 25]. A 50 mg single crystal with dimension about $5 \times 5 \times 1$ mm$^3$ was selected for neutron diffraction experiment, which was performed on hot-neutron four-circle diffractometer HEIDI at FRM II, Garching (Germany). A Cu (220) monochromator was selected to produce a monochromatic neutron beam with the wavelength at 0.868 Å. An Er filter was used to minimize the $\lambda/2$ contamination. Single crystal sample was mounted on a thin aluminium holder inside a standard closed-cycle cryostat. The diffraction data were collected using a $^3$He single detector at different temperatures from 300 K down to 2.5 K. A fine collimation ($\sim 15^\circ$) in front of the sample and a narrow opening of the detector slits were adopted to achieve a sufficient resolution, in order to determine precisely the structural splitting due to orthorhombic twinning and magnetic modulation wave vectors. To ensure the inclusion of the contributions from all possible twinned domains, the integrated intensities were collected with the setup adopting a 60$^\circ$ collimation and an angular opening of both horizontal and vertical detector slits set at 4.5 degree. Furthermore, the integrated intensities for the reflections with $2\theta > 60^\circ$ and $2\theta < 60^\circ$ were obtained respectively via the $\theta-2\theta$ and the rocking-curve scans. The obtained data used for the structural refinements were normalized by monitor counts and corrected for the Lorentz factor. DATAP program is used to carry out absorption correction by considering the size and shape of crystal [31]. The absorption coefficient $\mu$ is calculated to be 2.61 mm$^{-1}$ and the transmission factors are deduced to be only in the range from 2.1% up to 14.2% due to the extremely strong absorption. Determination of both the nuclear and magnetic structures was performed by using the FULLPROF program suit [32]. The scale factor derived from the crystal structure refinement was used to determine

![Graph](image-url)
plane and formed the domain pairs (D1 and D2), while another two shared the (110) plane (D3 and D4). In principle, it is possible to observe single peak, two or three or four peaks depending on the selected reflections and the resolution of the instrument. In Fig. 1(c), the left and right peaks can be assigned to the contributions from the domains (D1+D3) and (D2+D4) respectively. Note that the ω-scan is performed with open detector slits. Two Gaussian peaks were used to fit the (400)ₜ and (040)ₜ reflections and the domain population ratio is estimated to be around 1:1 for the (h00) and (0k0) twins, i.e. D1+D3 ≈ D2+D4. The ω-scan of (220) is examined afterward with the (hk0) aligned in the horizontal scattering plane to obtain more detailed information about domain population (Fig. 1(d)). The occurrence of twinning and T-O structural phase transition can be confirmed from the clear presence of triple splitting of (220) nuclear reflection. Usually, the reflections with $h = k \neq 0$ are triply split in twinned orthorhombic lattice and the peak in the center is attributed to pairs that share the same (110) or (110) plane, while the peak at left and right sides corresponds to the rest two domains. In Fig. 1(d), it can be seen that all three peaks showed almost equal intensity. This strongly indicates that the domain population exists the following relationship: D1 ≈ D3+D4 ≈ D2. Hence the domain population for all those four different domain patterns can be determined roughly as 2:2:1:1. In order to investigate the distribution of nuclear reflection in reciprocal space and determine the lattice parameter accurately, two dimensional plot of (400)ₜ reflection is shown in Fig. 1 (g). The splitting of (400)ₜ can also be clearly seen. Totally 280 nuclear reflections were collected for nuclear structure refinement within the Fmmm space group. Several strong reflections were excluded from the refinement because of the significant extinction. All atoms were refined with the isotropic temperature factor. The refinement results of crystal structure are listed in Table 1. The lattice parameters are deduced to be $a = 5.537(2)$ Å, $b = 5.505(2)$ Å and $c = 12.057(2)$ Å at 2.5 K, which are in good agreement with a previous report [35].

To clarify the magnetic structure of EuFe₂As₂ at low temperature, the sample was cooled to 2.5 K, which is well below the reported Fe²⁺ and Eu²⁺ magnetic ordering temperatures. Considering the existence of the twined (h00) and (0k0) domains, extensive search of magnetic reflections was performed in the $a^*c^*$ reciprocal space as schematically illustrated in Fig. 2(a). Additional search was also performed in the (hhl) reciprocal plane. Fig. 2(b) shows three typical long l scans in the reciprocal space where in addition to the expected nuclear reflections, two sets of magnetic superstructure reflections can be clearly identified with two magnetic propagation wave vectors (1,0,1) and (0,0,1) respectively. As an example, Q scan of (101)ₘ magnetic reflection is plotted in Fig. 3(a) and the same scan at 200 K is also plotted together for comparison. In Fig. 3(b), the 0-2θ scan of nuclear (002)ₙ and magnetic (003)ₘ reflections show the same peak center, which indicates that the magnetic structure is commensurate in nature. The contour map of (103)ₘ and (401)ₘ reflections fully illustrated the intensity distribution as shown

III. RESULTS AND DISCUSSION

First of all, the crystal structure of EuFe₂As₂ is described within the framework of tetragonal symmetry at 300 K. The ω scans of selected nuclear (220)ₜ and (200)ₜ reflections with mosaic width of ~0.22° are shown in Fig. 1 (a) and (b), which indicate the good quality and homogeneity of the single crystal. Upon cooling down, a splitting is observed for orthorhombic (400)ₜ and (040)ₜ reflections (Fig. 1(c)). Note that those two reflections are corresponding to the (220)ₜ in tetragonal setting according to the Tetragonal-Orthorhombic symmetry relation. The observed splitting of (400)ₜ is the indication of T-O structural transition and accompanied twinning configuration due to the interchange of the orthorhombic $a$ and $b$ axes. It is known that twinning in orthorhombic structure will result in four different domain patterns [33,34], as illustrated in Fig. 1 (e). Two of domains shared the same (110)
in Fig. 3(c) and Fig. 3(e). As already discussed, the contour map of (400)\(\nu\) nuclear reflection (Fig. 1(g)) clearly shows two reflections attributed to the (h00) and (0k0) twins. Two peak centers with \(k = 3.967\) and 4.01 can be obtained by fitting the \(Q\) scan of (400)\(\nu\) reflection (Fig. 1(h)). In Fig. 3(d), the \(Q\) scan of (103)\(\mu\) reflection can be fitted by a single Gaussian function with \(k = 0.991\). This strongly indicates that the (h00) type reflections (with \(h\) and \(l\) equal to odd number) are associated with the (h00) domain and they can thus be described with the propagation wave vector \(\mathbf{k} = (1,0,1)\). This wave vector is exactly the same as observed in other ‘122’ pnictides, such as BaFe\(_{2}\)As\(_{2}\) [13] and CaFe\(_{2}\)As\(_{2}\) [14], which is related to the AFM order of Fe\(^{2+}\) moments. The magnetic structure refinement was then carried out to determine the magnitude and direction of Fe\(^{2+}\) moment. The magnetic structure with Fe saturation moment of 0.98(8) \(\mu_B\) aligned along the long \(a\) axis is deduced. Note that the origin of AFM order in FeAs-based pnictides is still a matter of controversy. It is argued that the AFM order of Fe\(^{2+}\) may arise from the SDW order due to the Fermi surface instability under the itinerant model

![Diagram](image1.png)

**FIG. 3:** (Color online) (a) The comparison of the \(Q\) scan of (101)\(\mu\) magnetic reflection at 2.5 and 200 K. The (101)\(\mu\) reflection is observed in \(k\) scan because of the existence of twining. (b) The \(\theta-2\theta\) scan of (003)\(\nu\) nuclear and (003)\(\mu\) magnetic reflections at 2.5 K, the same scan of (003)\(\mu\) magnetic reflection at 300 K is also plotted for comparison. (c) The contour map shows the \(Q\) dependence of the (103)\(\mu\) magnetic reflection. (d) \(Q\) scan of (103)\(\mu\) magnetic reflection. (e) The contour map of (041)\(\mu\) magnetic reflection indicates the contribution of the magnetic reflection of Eu magnetic sublattice. (f) \(Q\) scan of (041)\(\mu\) magnetic reflection.

![Diagram](image2.png)

**FIG. 4:** (Color online) (a)-(e) Omega scans of series of (02l) (with \(l = \) odd) reflections at 2.5 K. The integrated intensities of (20l) and (02l) can be obtained by fitting the curves with two Gaussian functions. (f) The ratio between (20l) and (02l) reflections shows good agreement with the calculated value.

**TABLE I:** Refined results of the crystal and magnetic structures for EuFe\(_{2}\)As\(_{2}\) at 2.5 K (space group: \(\textit{Fmmm}, Z = 4\)).

| Atom/site | \(x\) | \(y\) | \(z\) | \(B(\text{Å}^2)\) |
|-----------|------|------|------|----------------|
| Eu (4a)   | 0    | 0    | 0    | 0.81(3)       |
| Fe (8f)   | 0.25 | 0.25 | 0.25 | 0.26(3)       |
| As (8i)   | 0    | 0    | 0.363(5) | 0.25(3)       |
|            | \(a, b, c (\text{Å})\): 5.537(2), 5.505(2), 12.057(2) |
|            | Number of reflections (Nuclear): 280 |
|            | \(RF^2, RF^{2\text{W}}, RF\%, \chi^2\) Nuclear: 9.34, 9.67, 6.22, 7.1 |
|            | Number of reflections (Magnetic): 228 |
|            | \(RF^2, RF^{2\text{W}}, RF\%, \chi^2\) Magnetic: 9.42, 7.68, 6.53, 5.7 |

While other evidences support that the AFM order has a local moment origin as in Mott insulator [37, 38], such as the parent compound of high \(T_c\) cuprates. Recent spin wave excitation study on CaFe\(_{2}\)As\(_{2}\) suggests that the magnetism of iron arsenide might be resulted from a complicated mixture of localized and itinerant properties and it should be understood by considering both the localized and itinerant electrons [39]. Consequently, the magnetic reflections with a propagation wave vector \(\mathbf{k} = (0,0,1)\) (with \(h\) even and \(l\) odd) are due to the long range order of the localized Eu\(^{2+}\) moments. However, the moment direction of Eu\(^{2+}\) moments is still indeterminate.
Symmetry analysis based on the representation theory indicates that the magnetic representation $\Gamma$ for magnetic Eu$^{2+}$ on 4$a$ site is decomposed into three one dimensional irreducible representations: $\Gamma_1, \Gamma_2$ and $\Gamma_3$. The Eu$^{2+}$ moments are aligned in the $c$, $a$ or $b$ direction according to those three representations. The observation of nonzero intensity of $(00l)$ (with $l =$ odd) reflections clearly exclude the representation $\Gamma_1$. The $\omega$ scans on several $(hk0)_M$ (with both $h$ and $k =$ odd) reflections also exhibit considerable intensity. Thus, the moment of Eu$^{2+}$ is expected to be aligned either along the $a$ or $b$ direction in the $ab$ plane. The $Q$ scan on $(041)_M$ reflection (Fig. 3(f)) giving a peak position of $k = 4.01$, which is exactly equal to the larger $k$ value of $(400)_O$ nuclear reflection. Therefore, the moment direction of Eu$^{2+}$ can be determined as along the $a$ direction since the intensity ratio between $(041)_M$ and $(401)_M$ magnetic reflections approximate equals to 73:1 for this arrangement. The structure mode is confirmed further by $\omega$ scan of series of $(02l)$ (with $l =$ odd) reflections as shown in Fig. 4. Similar to some nuclear reflections, both $(20l)$ and $(02l)$ magnetic reflections was detected due to the twinning configuration. However, the intensity ratio between $(20l)$ and $(02l)$ changes gradually with the change of the angle between the scattering plane and the $c$ axis. The calculated intensity ratio of $(20l)/(02l)$ for different $l$ are plotted in Fig. 4(f) and it agrees well with the observed values which derived from the $\omega$ scans directly. By taking into account of twinning components properly, the refinement on Eu$^{2+}$ magnetic sublattice was carried out with the aforementioned magnetic structure model. The calculated structure factors are plotted against those observed and shown in Fig. 5. The reliable agreement factors confirms the proposed magnetic structural model eventually, i.e. the Eu$^{2+}$ moment aligns along $a$ direction with the wave vector $\mathbf{k} = (0,0,1)$ and magnitude of 6.8(3) $\mu_B$. Thus the magnetic structure of EuFe$_2$As$_2$ is unambiguously determined as illustrated in Fig. 6. The moment direction of Eu$^{2+}$ is also consistent with our resonant x-ray scattering (RXS) measurement [40].

Fig. 5 shows the temperature dependence of the $(112)_M$ and $(003)_M$ magnetic reflections attributed to the ordering of Eu$^{2+}$ moments. The onset temperature of Eu$^{2+}$ magnetic order is deduced to be 19 K, which is in good agreement with previous report on electronic and magnetic measurements [24, 25]. The magnetic ordering temperature of Fe$^{2+}$ moment is estimated to be 190 K based on the temperature dependence of the $(101)_M$ and $(033)_M$ magnetic reflections (see Fig. 7(b)). The T-O structural phase transition also takes place at 190 K as revealed by the sharp change of full width at half maximum (FWHM) in $(040)_O$ nuclear reflection. First principle calculations suggest that the nearest and next nearest neighbor superexchange interactions between Fe ions lead to a frustrated magnetic ground state in pnictides with parallel and antiparallel arrangement of Fe spins in FeAs layer [41]. Usually, the magnetic frustration can be lifted by a structural distortion from low symmetry to high symmetry phase. This may be the origin of the strong coupling between the structural and magnetic phase transitions observed in EuFe$_2$As$_2$ and other iron pnictides [12, 13, 14].

Due to the localized nature of Eu 4$f$ state, the AFM coupling of Eu$^{2+}$ moments would be described by the indirect exchange, e.g. the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction as suggested by Ren et al. [30]. Besides of the Eu-Eu and Fe-Fe interactions, the strength of the interaction between the Eu and Fe magnetic sublattices is also an interesting issue. Similar to CaFe$_2$As$_2$, the SDW transition in EuFe$_2$As$_2$ can also be suppressed continuously by applying the pressure due to the weakening of nearest Fe-Fe exchange coupling [42]. Whereas the AFM ordering temperature of Eu sublattice does not change significantly even the compound exhibits the possible reentrant superconducting state. This may suggest the weak interaction between the Eu and Fe magnetic sublattices,
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