

Magnetic Form factor of detwinned single crystal of BaFe₂As₂

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We have performed neutron diffraction measurement on single crystal of a parent compound of iron-based superconductor BaFe₂As₂. In order to investigate in-plane anisotropy of magnetic form factor in the antiferromagnetic phase, the detwinned single crystal is used in the measurement. The observed magnetic form factors at reciprocal lattice points of $h0l$, $1k1$ and $10l$ are shown in Fig. 1 by closed circle, closed triangle and open circle, respectively. In the estimation of the magnetic form factor, the so-called stripe magnetic structure whose magnetic moment is away from a -axis in a - b plane by 10 degrees is assumed. The decrease with Q of the magnetic form factor at $h0l$ is more gradual than the decreases at $1k1$ and $10l$, indicating that the $3d$ electrons contributing to the magnetic moment have anisotropic distribution in a - b plane. The solid and dashed lines in the figure are the magnetic form factors calculated by assuming the polarized $3d_{yz}$ electrons with a fraction of 40 % and the polarized electrons in other four $3d$ orbitals with each fraction of 15 %. The calculated form factors can reproduce the observed ones. The obtained magnetic form factor and/or the distribution of the $3d$ electrons contributing to the magnetic moment, are qualitatively consistent with that suggested by the orbital ordering model.[1] Our results can lead to the understanding the in-plane anisotropy of the magnetic behaviors observed in the parent compounds of iron-based superconductors.[2]

References

[1] C. Lee, W. G. Yin and W. Ku, Phys. Rev. Lett. **103**, 267001 (2009).

[2] For example, J. Zhao et al., Nature Physics **5**, 555 (2009).

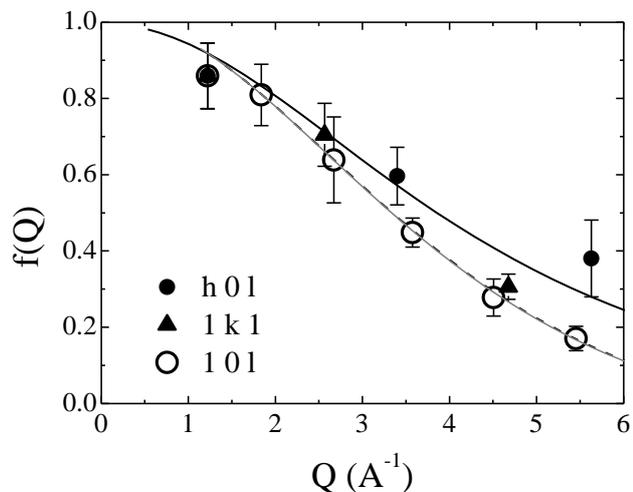


Fig. 1 Observed and calculated magnetic form factors of $h0l$, $1k1$, and $10l$ reflections.