Ab initio calculation of X-ray circular dichroism of magnetic chiral crystal using SPR-KKR program

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B20-type FeGe is a well-known chiral magnetic material that exhibits ferromagnetism and crystallographic chirality, and it belongs to crystal class 23. X-ray Magnetic Circular Dichroism (XMCD) and X-ray Natural Circular Dichroism (XNCD) are powerful tools for investigating magnetism and structural chirality, respectively. However, Goulon *et al.* reported that among non-centrosymmetric crystal classes 432 and 23 do not exhibit any observable XNCD signal [1]. This appears counter-intuitive, since B20-type FeGe possesses helical-like atomic arrangements along the [111] direction, which intuitively suggest the presence of structural chirality.

In this study, we numerically verify the absence of XNCD in crystal class 23 by performing numerical calculations of XNCD spectra using the Spin-Polarized Relativistic Korringa–Kohn–Rostoker (SPR-KKR) code [2]. Our results show that the XNCD spectrum of one prototypical Fe site of four Fe absorption sites (Fe1–Fe4) in a unit cell is in antiphase with the summed spectra of the remaining three Fe sites, leading to a complete cancellation of the XNCD intensity. Furthermore, we show that this phase relationship among the spectra can be described by a second-order Legendre polynomial, reflecting the local C3 symmetry at the Fe sites. These results clarify the microscopic origin of the absence of XNCD in B20-type FeGe reported by Goulon *et al.*, demonstrating that site-resolved XNCD signals cancel exactly due to symmetry relations among the Fe sites. Furthermore, we shall introduce cross densities of states (X-DOS), which are analogous to those of the XNCD spectrum [3].

References

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