Master thesis

修士論文

Title

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Abstract

The magneto electric effect has been attracted much attention. The ME effect is . The ME effect can be However can not used due to its smallness and temperature.

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Introduction

1.1 Citation and Chemical Formula

Citation [?] Chemical Formula Cr_2O_3

Method

To elucidate the microscopic mechanism of the ME effect, an effective model

2.1 Equation

2.1.1 Equation

equation

$$E_{\text{total}}(u_m, e_i) = E_0 + E_{\text{phonon}}(u_m) + E_{\text{spin}}(u_m, e_i). \tag{2.1}$$

2.2 Figure

2.2.1 Figure

FIGURE

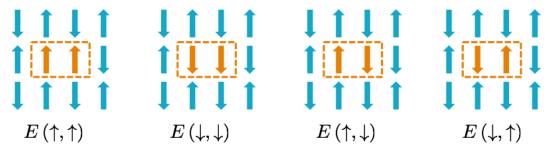


Figure 2.1: The four different spin configurations

4 Chapter 2 Method

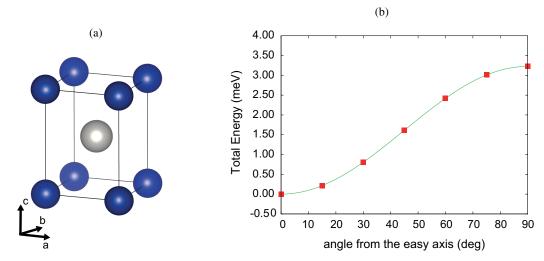


Figure 2.2: (a) The unit cell of CoPt. (b) Magnetic anisotropic energy of CoPt.

Results

For $\mathrm{Cr_2O_3}$ we determine the parameters of the effective Heisenberg model introduced in Chapter.2

3.1 Table

3.1.1 Table

Chapter reference Fig2.2.

	A_{2u} r	nodes		E_u m	odes	
LDA+U (this work)	407	574	311	447	562	635
PBE (Ref. [?])	388	522	297	427	510	610
Expt. (Ref. [?])	402	533	305	440	538	609

Table3.1: Phonon frequencies (cm⁻¹)

Conclusion

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Appendix A

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Acknowledgements

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