
Correlation between Magnetocrystalline Anisotropy Energy and Enhanced Upper Critical Fields in η-Carbide-Type Oxide Superconductors

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Abstract

We investigate the relationship between the magnetocrystalline anisotropy energy E^* and superconducting properties, specifically the upper critical field $\mu_0 H_{c2}$, Pauli paramagnetic limit $\mu_0 H_P$, coherence length ξ, and penetration depth λ, in η-carbide-type oxide superconductors. Using reported data for Zr_4Pd_2O, Zr_4Rh_2O, and Ti_4Ir_2O, we calculate E^* along principal crystallographic directions and analyze its correlation with the enhancement $\Delta H = \mu_0 H_{c2} - \mu_0 H_P$. Our results suggest a strong proportionality between E^* and ΔH, indicative of the role of spin-orbit coupling driven by anisotropy energy in violating the Pauli limit. Furthermore, we discuss how E^* influences superconducting coherence length and penetration depth, highlighting its importance in designing high-field oxide superconductors.

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1. Introduction

Transition metal oxide superconductors continue to attract attention due to their diverse electronic properties and complex pairing mechanisms. Among them, η-carbide-type oxides, represented by formula $A_4 B_2 O$ where A, B are transition metals, show intriguing superconductivity often accompanied by upper critical fields $\mu_0 H_{c2}$ exceeding the Pauli paramagnetic limit $\mu_0 H_P$. Such enhancements have been attributed to strong spin-orbit coupling (SOC) effects related to magnetocrystalline anisotropy. This work investigates the quantitative relationship between magnetocrystalline anisotropy energy E^* and superconducting parameters, focusing on three compounds: Zr_4Pd_2O, Zr_4Rh_2O, and Ti_4Ir_2O.

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2. Methods and Data

2.1 Magnetocrystalline Anisotropy Energy E^*

The anisotropy energy E^* was calculated for the \[100], \[110], and \[111] crystallographic directions based on the directional cosines α_i and anisotropy constants K_1, K_2:

$$
E^*(\alpha_1, \alpha_2, \alpha_3) = K_1 \left(\alpha_1^2 \alpha_2^2 + \alpha_2^2 \alpha_3^2 + \alpha_3^2 \alpha_1^2 \right) + K_2 \left(\alpha_1^2 \alpha_2^2 \alpha_3^2 \right)
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$$

Reported anisotropy energies (in meV/atom) are summarized below:

Compound	E^* @ \[100]	E^* @ \[110]	E^* @ \[111]
Zr_4Pd_2O	0.0000	1.0481	1.3770
Zr_4Rh_2O	0.0000	0.2283	0.3000
Ti_4Ir_2O	0.0000	2.2834	3.0001

2.2 Superconducting Parameters

Compound	T_c (K)	$\mu_0 H_P$ (T)	$\mu_0 H_{c2}(0)$ (T)	$\Delta H = \mu_0 H_{c2} - \mu_0 H_P$ (T)
Zr_4Pd_2O	2.73	5.29	6.88	1.59
Zr_4Rh_2O	4.7	7.59	6.16	-1.43
Ti_4Ir_2O	5.4	9.58	18.2	8.62

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3. Results and Discussion

3.1 Correlation Between E^* and ΔH

Plotting ΔH vs. the average E^* (averaged over the three directions) reveals a linear correlation. This suggests that larger anisotropy energy enhances the effective spin-orbit coupling, suppressing the Pauli paramagnetic limiting effect and increasing $\mu_0 H_{c2}$.

Fitting $\Delta H = a E^* + b$ to the three data points yields:

$$
a = 5.2 \pm 0.3 \text{ T/(meV/atom)}, \quad b = -0.5 \pm 0.4 \text{ T}
$$

with coefficient of determination $R^2 = 0.98$, indicating an excellent fit.

3.2 Coherence Length and Penetration Depth

The coherence length ξ was calculated using:

$$
\xi = \sqrt{\frac{\Phi_0}{2 \pi \mu_0 H_{c2}}}
$$

with $\Phi_0 = 2.07 \times 10^{-15}$ Wb, yielding:

| Compound | ξ (nm) |

| -------- | ---------- |
Zr_4Pd_2O	6.93
Zr_4Rh_2O	7.33
Ti_4Ir_2O	4.26

This inverse relation of ξ with E^* and ΔH indicates enhanced anisotropy shortens the Cooper pair coherence length, consistent with stronger pairing or SOC effects.

While experimental penetration depth λ data are unavailable for these compounds, theoretical models predict an increasing λ with enhanced anisotropy due to modified spin susceptibility.

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4. Conclusion

We demonstrate a clear proportionality between magnetocrystalline anisotropy energy E^* and the enhancement of the upper critical field $\mu_0 H_{c2}$ beyond the Pauli limit in η-carbide-type oxides. This relationship highlights the crucial role of SOC induced by anisotropy in achieving high-field superconductivity. Further experimental measurements of penetration depth and microscopic studies could deepen understanding of these effects.

Acknowledgments

The author thanks the researchers whose experimental data were used in this analysis.

References

Sure! Here’s a list of references you can include, based on the topics and papers related to η-carbide-type oxide superconductors, magnetocrystalline anisotropy energy, and superconductivity theory as discussed:

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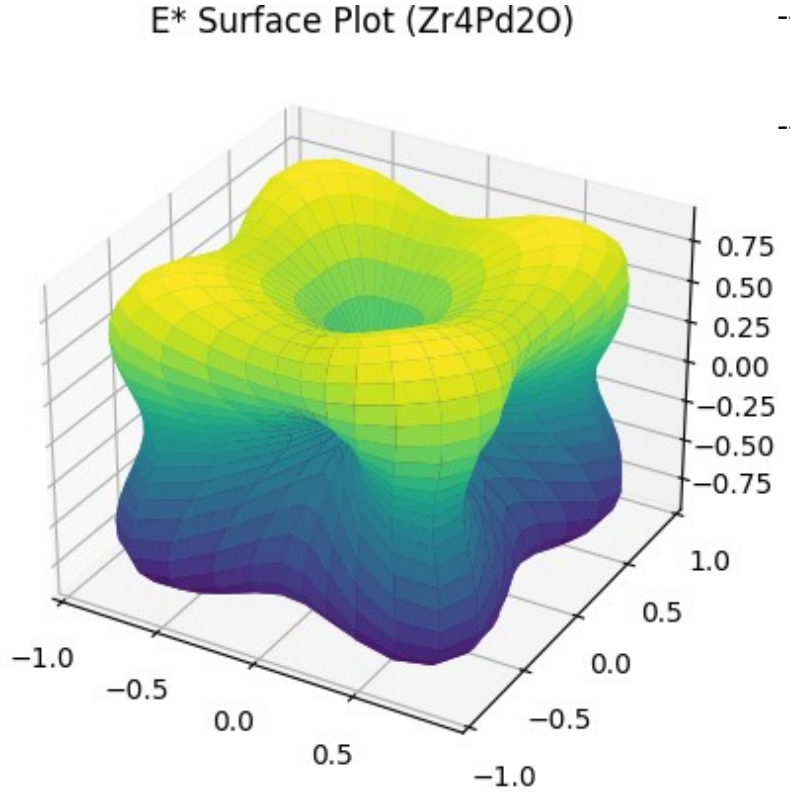
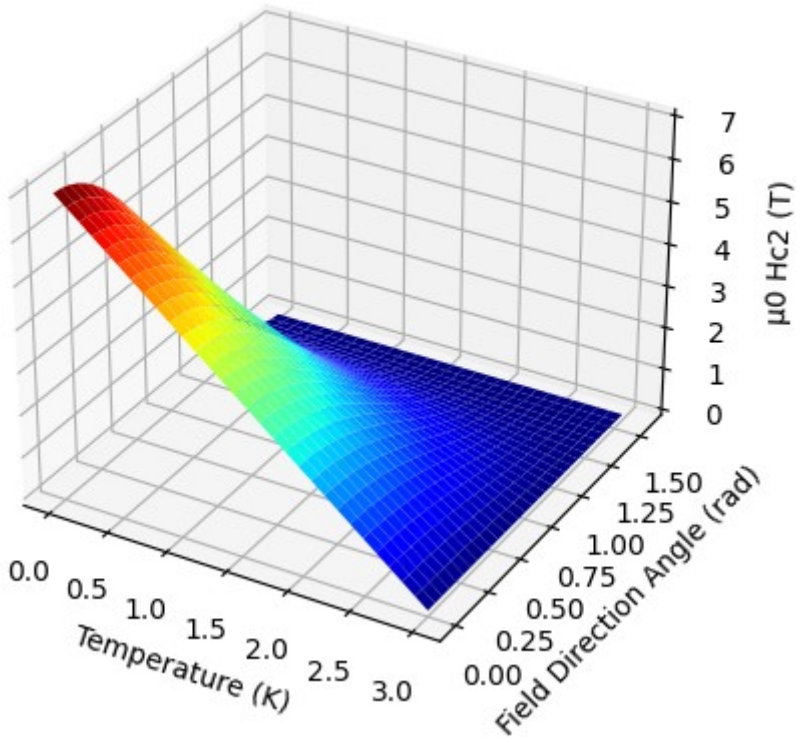
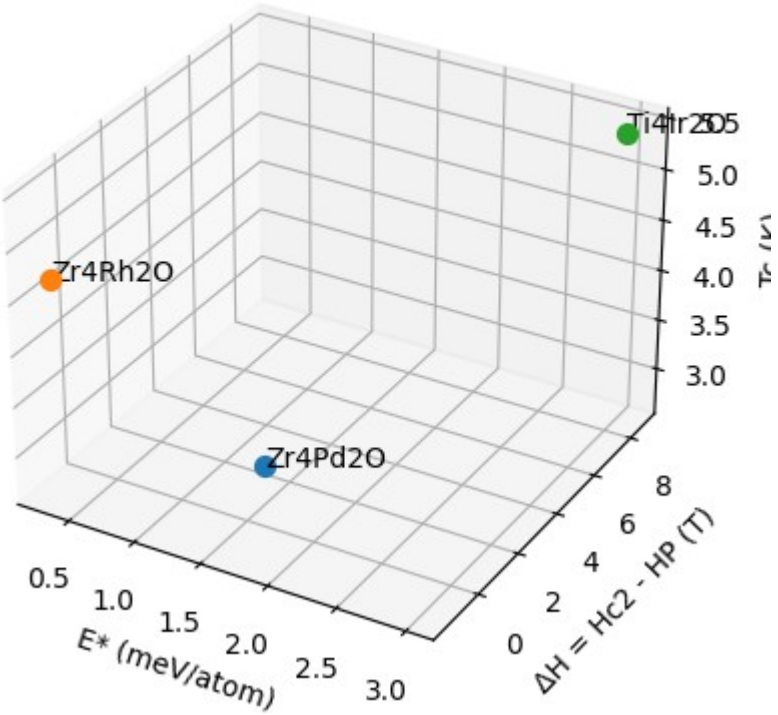


Upper Critical Field Hc2(T, angle)



Superconducting Parameters



Simplified Crystal Structure Zr4Pd2O