Magnetoelastic effect and strain induced anisotropy in cubic materials

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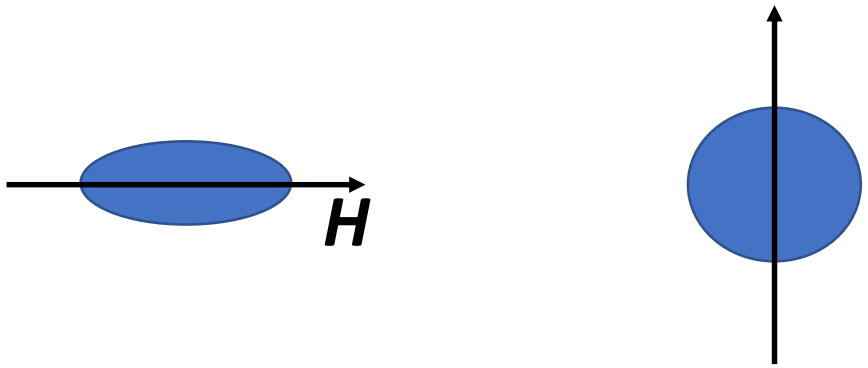
Xiaoshan Xu

Reference: Modern Magnetic Materials: Principles and Applications by R. C. O'Handley (2000).

Magnetoelastic effect and magnetostrictive effect

- Magnetoelastic effect
  - Change of magnetic properties (susceptibility and anisotropy due to strain ***e***)

- Magnetostriction
  - Shape change when a field (***H***) is applied (magnetized)
  - The change is typically very small (Fe, Co, Ni ≈ 50E-6, CoFe2O4 ≈ 500E-6)



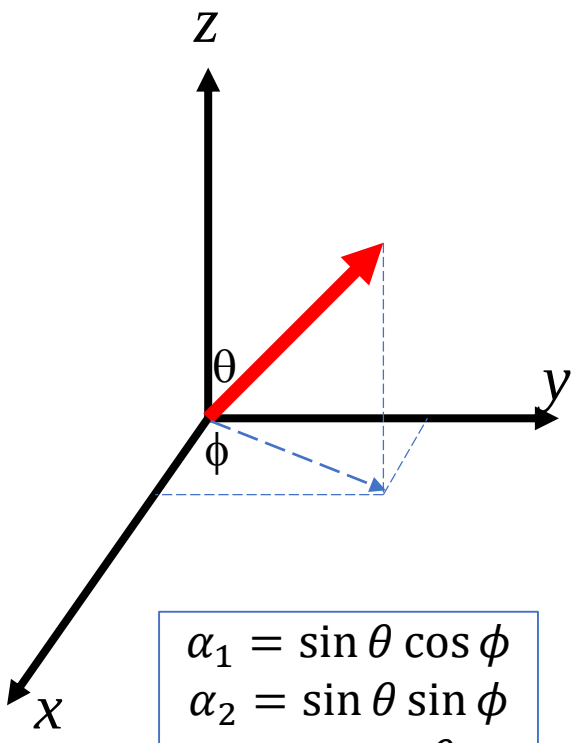
Landau theory of free energy for cubic material

$$U = U_M + U_E + U_{ME}$$

$$U_M = K_1(\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_3^2\alpha_1^2)$$

$$U_{ME} = B_1\left(\alpha_1^2 e_{xx} + \alpha_2^2 e_{yy} + \alpha_3^2 e_{zz}\right) + B_2\left(\alpha_1\alpha_2 e_{xy} + \alpha_2\alpha_3 e_{yz} + \alpha_3\alpha_1 e_{zx}\right)$$

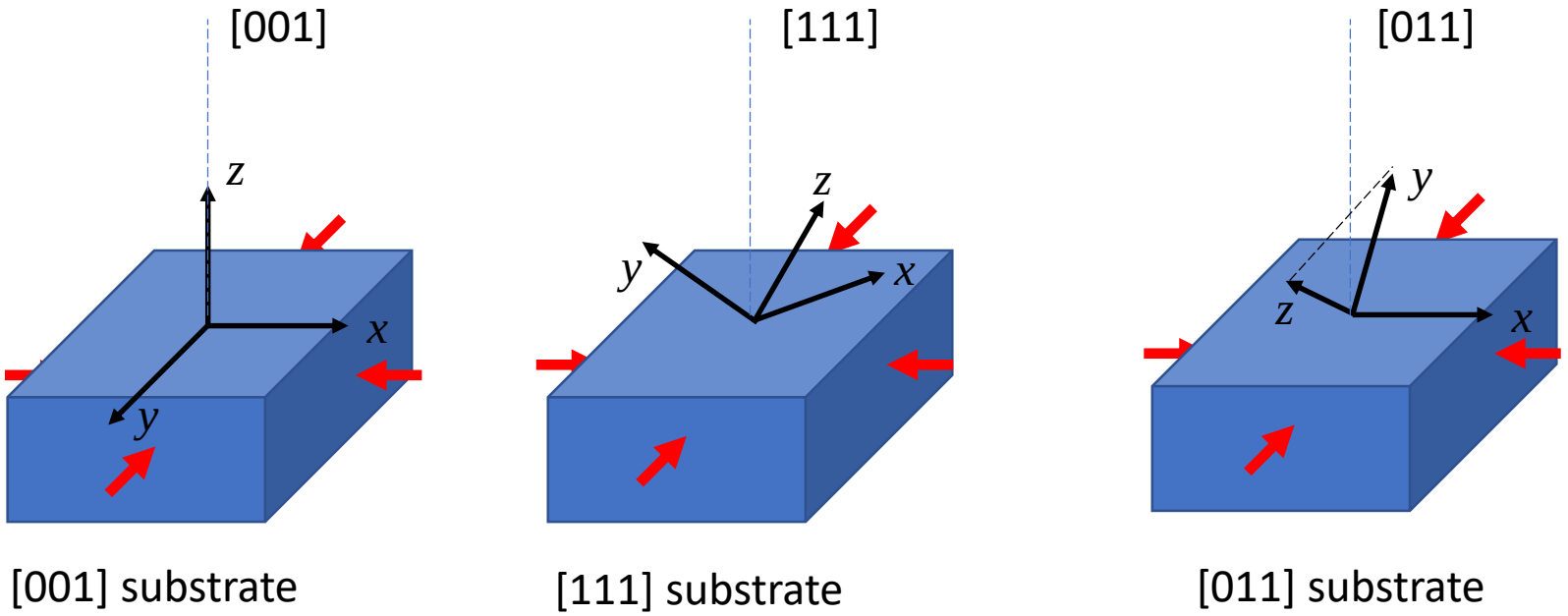
$$U_E = \frac{1}{2}c_{11}\left(e_{xx}^2 + e_{yy}^2 + e_{zz}^2\right) + c_{12}\left(e_{xx}e_{yy} + e_{xx}e_{zz} + e_{yy}e_{zz}\right) + \frac{1}{2}c_{44}\left(e_{xy}^2 + e_{yz}^2 + e_{zx}^2\right)$$



$$\alpha_1 = \sin\theta\cos\phi$$
$$\alpha_2 = \sin\theta\sin\phi$$
$$\alpha_3 = \cos\theta$$
$$\alpha_1^2 + \alpha_2^2 + \alpha_3^2 = 1$$

Considering magnetoelastic effect

$$U = U_M + U_{ME}$$
$$= K_1(\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_3^2\alpha_1^2) + B_1\left(\alpha_1^2 e_{xx} + \alpha_2^2 e_{yy} + \alpha_3^2 e_{zz}\right)$$
$$+ B_2\left(\alpha_1\alpha_2 e_{xy} + \alpha_2\alpha_3 e_{yz} + \alpha_3\alpha_1 e_{zx}\right)$$



No strain

- Strain: $e_{xx} = e_{yy} = e_{zz} = e_{xy} = e_{yz} = e_{zx} = 0$
- Free energy:

$$U = K_1(\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_3^2\alpha_1^2)$$
$$= K_1(\alpha_1^2 + \alpha_2^2 - \alpha_1^4 - \alpha_2^4 - \alpha_1^2\alpha_2^2)$$

- Taking first derivative,

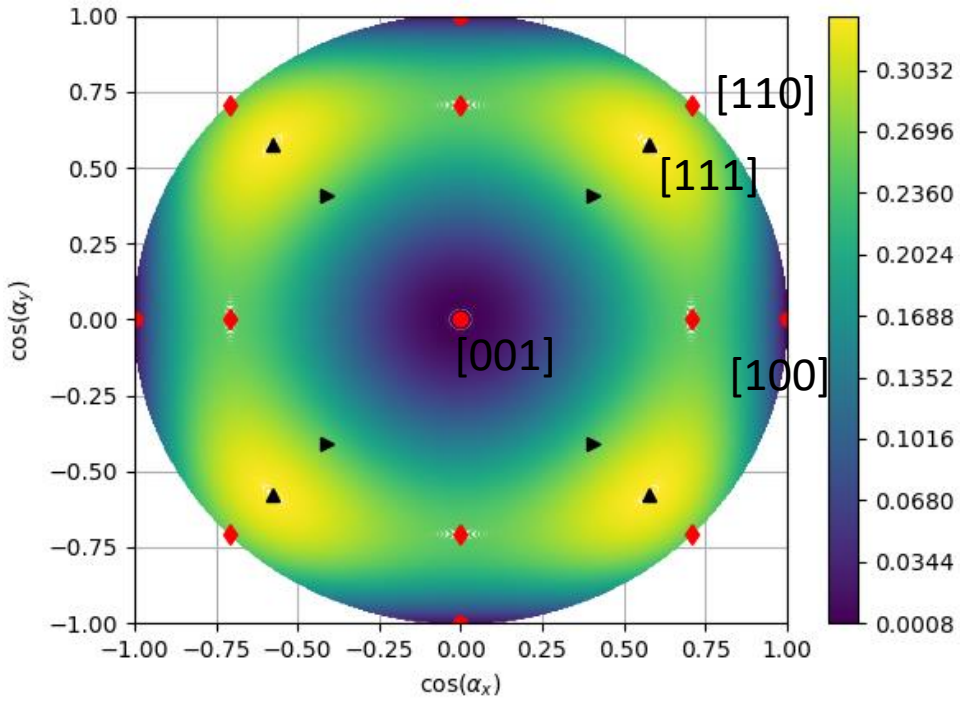
$$\frac{\partial U}{\partial \alpha_1} = K_1(2\alpha_1 - 4\alpha_1^3 - 2\alpha_1\alpha_2^2) = 0$$
$$\frac{\partial U}{\partial \alpha_2} = K_1(2\alpha_2 - 4\alpha_2^3 - 2\alpha_2\alpha_1^2) = 0$$

$$\boxed{\begin{aligned} 2\alpha_1(1 - 2\alpha_1^2 - \alpha_2^2) &= 0 \\ 2\alpha_2(1 - 2\alpha_2^2 - \alpha_1^2) &= 0 \end{aligned}}$$

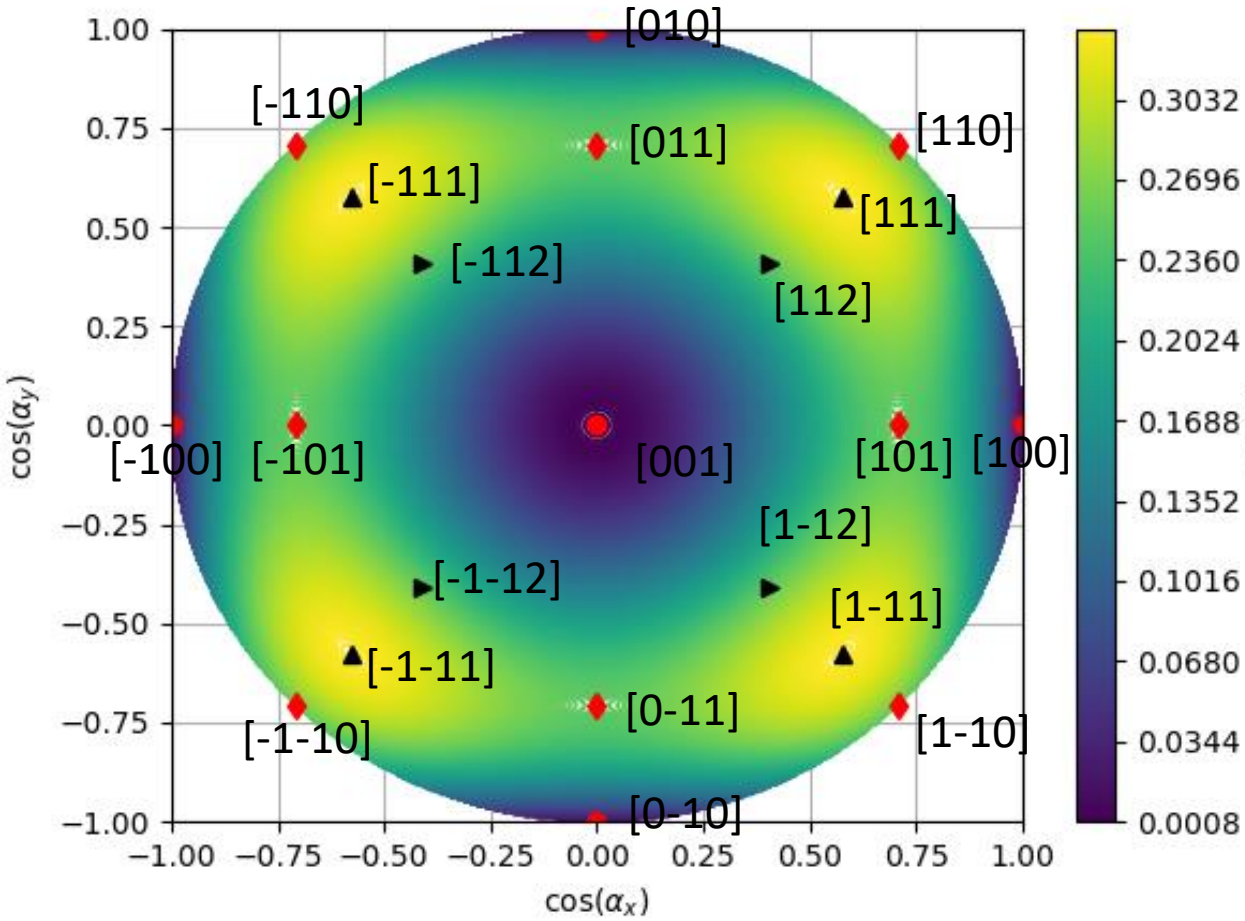
- And 2nd derivative,

$$\frac{\partial^2 U}{\partial \alpha_1^2} = K_1(2 - 12\alpha_1^2 - 2\alpha_2^2)$$
$$\frac{\partial^2 U}{\partial \alpha_2^2} = K_1(2 - 12\alpha_2^3 - 2\alpha_1^2)$$

$$2\alpha_1(1-2\alpha_1^2-\alpha_2^2)=0$$
$$2\alpha_2(1-2\alpha_2^2-\alpha_1^2)=0$$

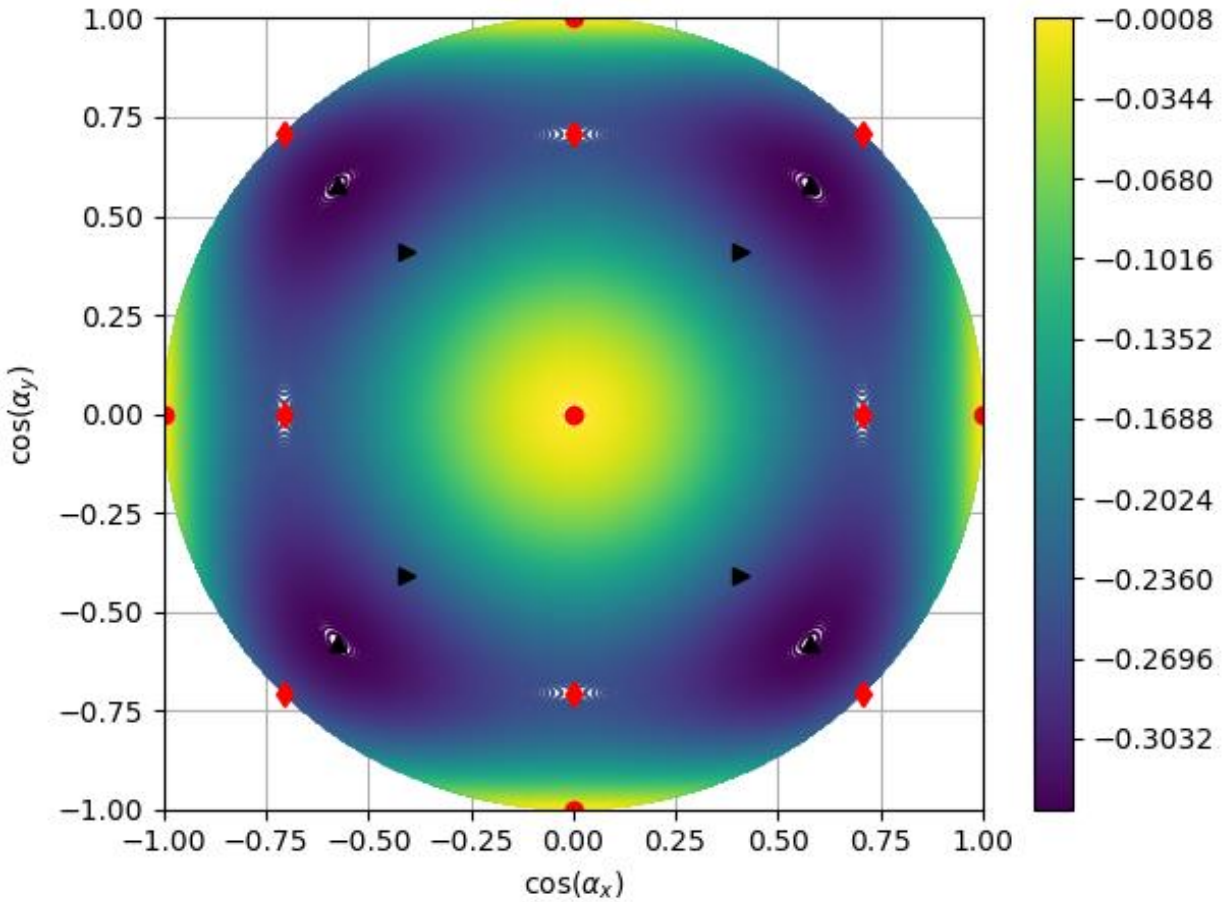


#	α_1	α_2	$\frac{\partial^2 U}{\partial \alpha_1^2}$	$\frac{\partial^2 U}{\partial \alpha_2^2}$	axis	$K_1 > 0$	$K_1 < 0$
1	0	0	$2K_1$	$2K_1$	[0, 0, 1]	Easy axis	Hard axis
2	0	$\pm\frac{1}{\sqrt{2}}$	K_1	$-4K_1$	[0±, 1, ±1]	Saddle	saddle
3	$\pm\frac{1}{\sqrt{2}}$	0	$-4K_1$	K_1	[±1, 0, ±1]	saddle	Saddle
4	$\pm\frac{1}{\sqrt{3}}$	$\pm\frac{1}{3}$	$-\frac{8}{3}K_1$	$-\frac{8}{3}K_1$	[±1,±1,±1]	Hard axis	Easy axis



$K_1 > 0$

Fe, CoFe2O4, NiCo2O4



$K_1 < 0$

Ni

[001] strain

- Strain: $e_{xy} = e_{yz} = e_{zx} = 0, e_{xx} < 0, e_{yy} < 0, e_{zz} > 0, |e_{xx}| = |e_{yy}| = |e_{zz}| = e$
- Free energy:

$$U = K_1(\alpha_1^2 + \alpha_2^2 - \alpha_1^4 - \alpha_2^4 - \alpha_1^2\alpha_2^2) + eB_1(-2\alpha_1^2 - 2\alpha_2^2 + 1)$$

- Taking first derivative,

$$\frac{\partial U}{\partial \alpha_1} = K_1(2\alpha_1 - 4\alpha_1^3 - 2\alpha_1\alpha_2^2) - 4eB_1\alpha_1 = 0$$

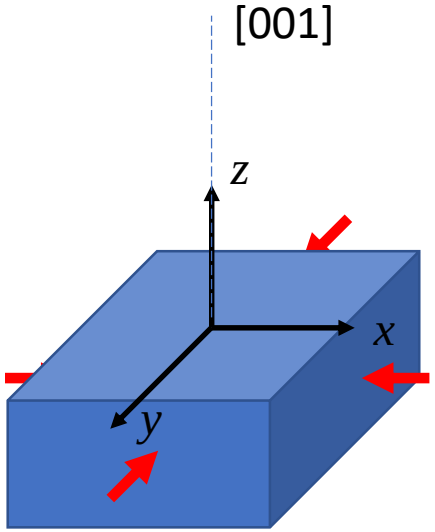
$$\frac{\partial U}{\partial \alpha_2} = K_1(2\alpha_2 - 4\alpha_2^3 - 2\alpha_2\alpha_1^2) - 4eB_1\alpha_2 = 0$$

$$\boxed{\begin{aligned} 2\alpha_1(K_1 - 2eB_1 - 2K_1\alpha_1^2 - K_1\alpha_2^2) = 0 \\ 2\alpha_2(K_1 - 2eB_1 - 2K_1\alpha_2^2 - K_1\alpha_1^2) = 0 \end{aligned}}$$

- And 2nd derivative,

$$\frac{\partial^2 U}{\partial \alpha_1^2} = K_1(2 - 12\alpha_1^2 - 2\alpha_2^2) - 4eB_1$$

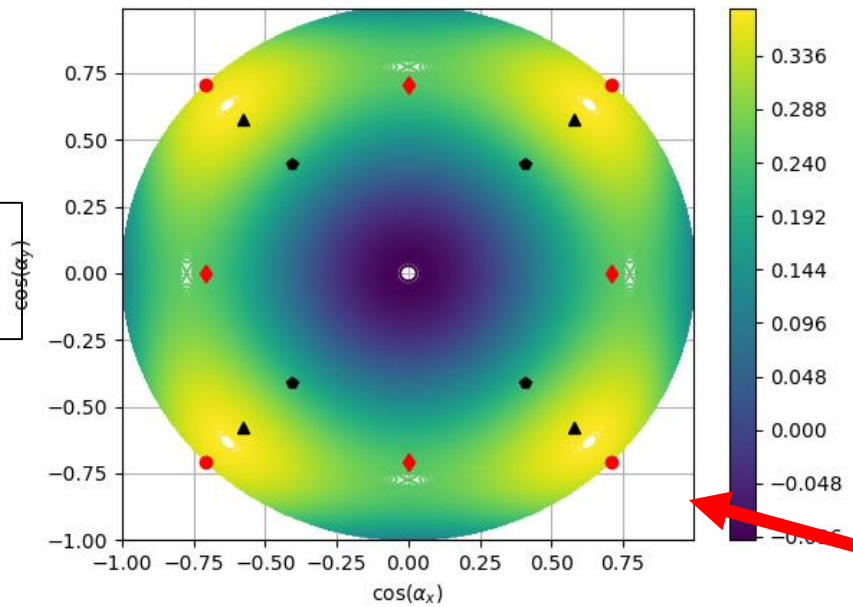
$$\frac{\partial^2 U}{\partial \alpha_2^2} = K_1(2 - 12\alpha_2^3 - 2\alpha_1^2) - 4eB_1$$

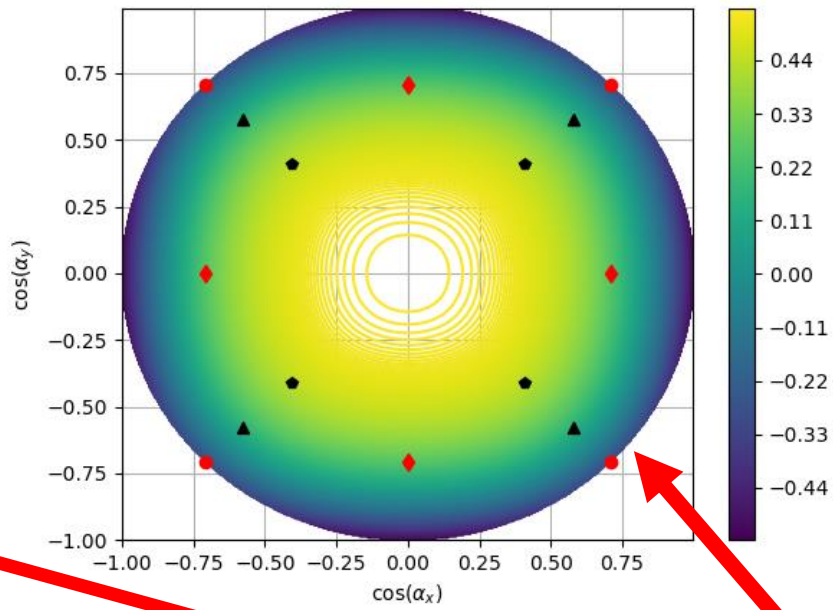


[001] substrate

$$2\alpha_1(K_1 - 2eB_1 - 2K_1\alpha_1^2 - K_1\alpha_2^2) = 0$$
$$2\alpha_2(K_1 - 2eB_1 - 2K_1\alpha_2^2 - K_1\alpha_1^2) = 0$$

$B_1 < 0$, if [001] is the global easy axis.





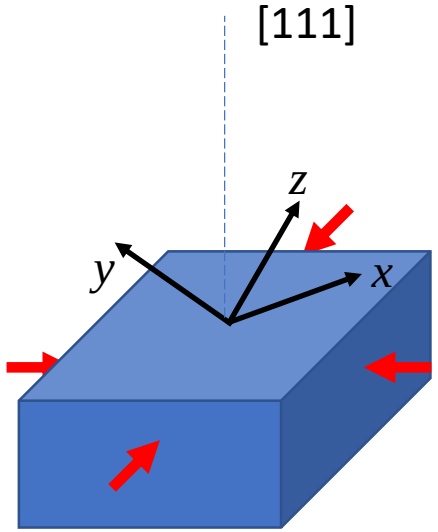
#	α_1	α_2	$\frac{\partial^2 U}{\partial \alpha_1^2}$	$\frac{\partial^2 U}{\partial \alpha_2^2}$	axis	$K_1 - 2eB_1 > 0$	$K_1 - 2eB_1 < 0$
1	0	0	$2(K_1 - 2eB_1)$	$2(K_1 - 2eB_1)$	[0, 0, 1]	Easy	Hard
2	0	$\pm\sqrt{\frac{K_1 - 2eB_1}{2K_1}}$	$K_1 - 2eB_1$	$-4(K_1 - 2eB_1)$	[0±, 1, ±1+δ]	saddle	saddle
3	$\pm\sqrt{\frac{K_1 - 2eB_1}{2K_1}}$	0	$-4(K_1 - 2eB_1)$	$K_1 - 2eB_1$	[±1, 0, ±1+δ]	saddle	Saddle
4	$\pm\sqrt{\frac{K_1 - 2eB_1}{3K_1}}$	$\pm\sqrt{\frac{K_1 - 2eB_1}{3K_1}}$	$-\frac{8(K_1 - 2eB_1)}{3}$	$-\frac{8(K_1 - 2eB_1)}{3}$	[±1,±1,±(1+δ)]	hard	easy

[111] strain

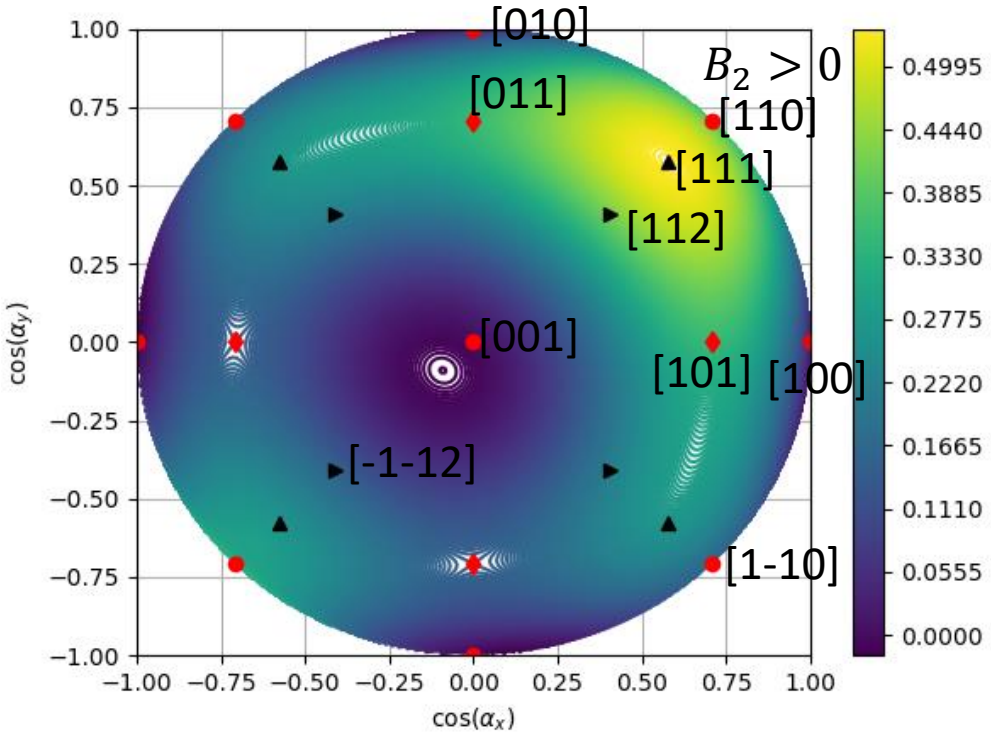
- Strain: $e_{xy} > 0, e_{yz} > 0, e_{zx} > 0$
- Free energy:

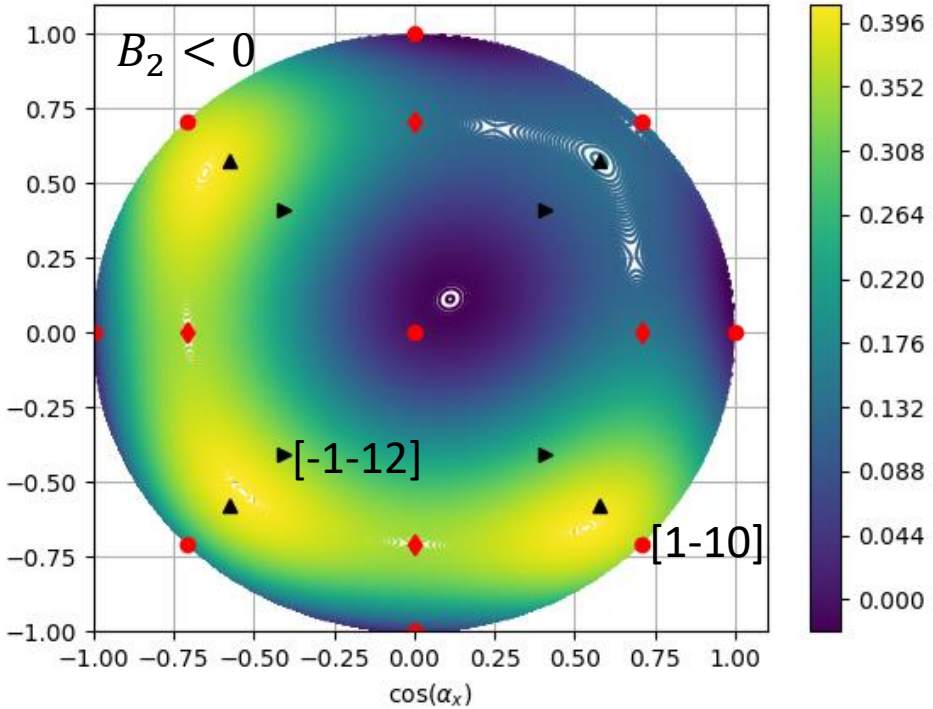
$$U = K_1(\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_3^2\alpha_1^2) + B_2(\alpha_1\alpha_2|e_{xy}| + \alpha_2\alpha_3|e_{yz}| + \alpha_3\alpha_1|e_{zx}|)$$

$B_2 < 0$, if [111] is not the global hard axis.

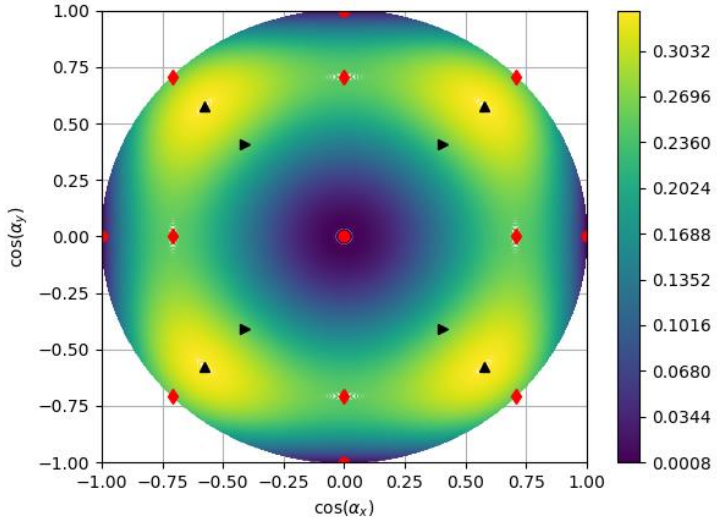


[111] substrate



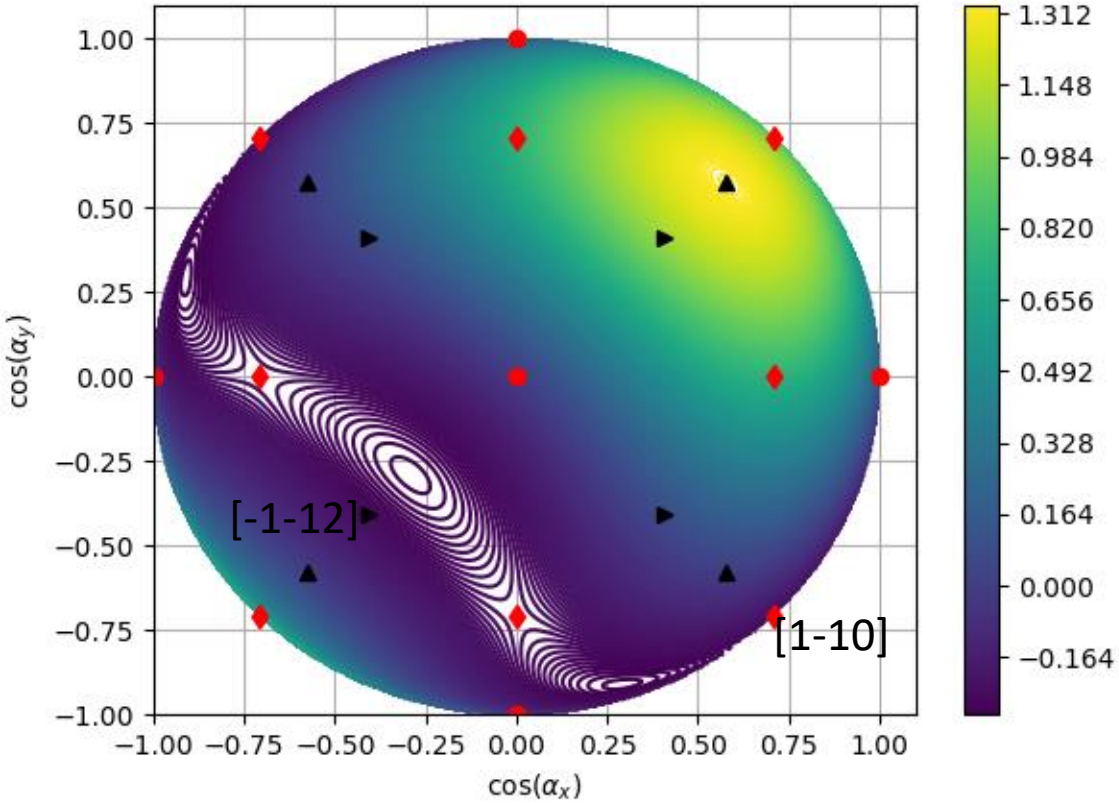


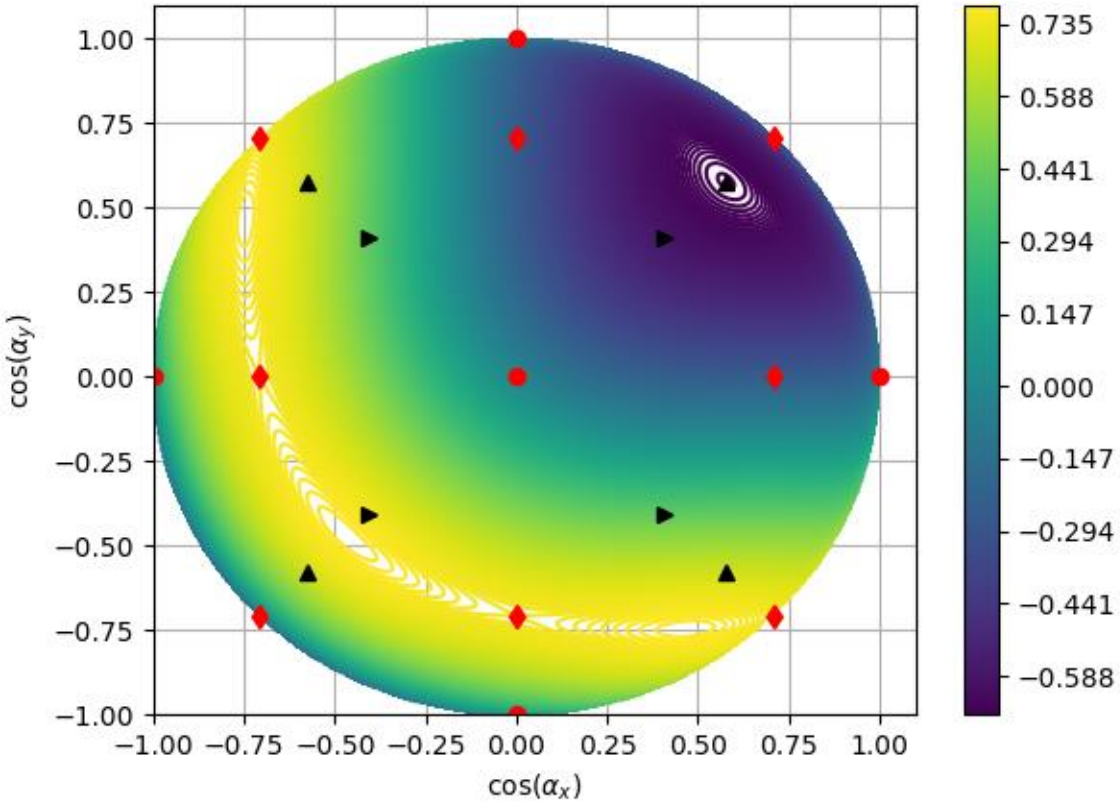
[111] strain



Large In-plan isotropy

small In-plan isotropy

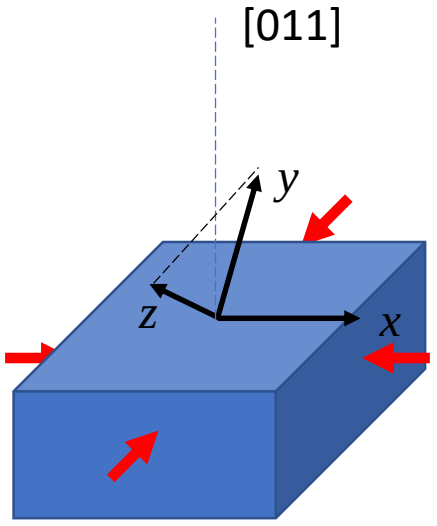




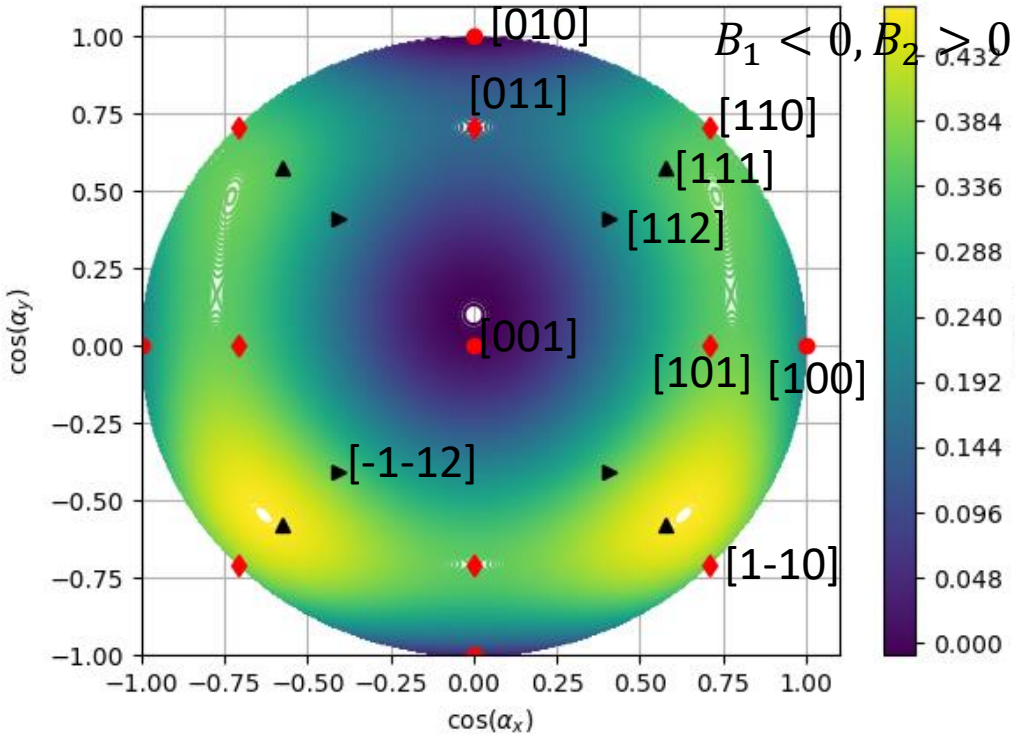
[011] strain

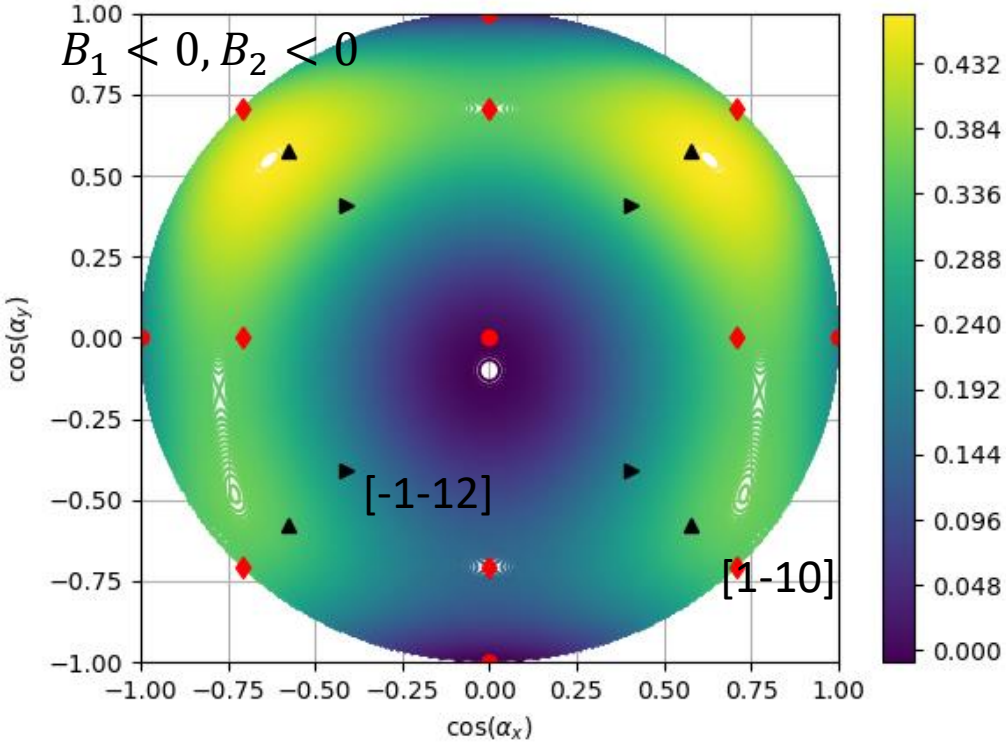
- Strain: $e_{xx} < 0, e_{yz} > 0.$
- Free energy:

$$U = K_1(\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_3^2\alpha_1^2) - B_1\alpha_1^2|e_{xx}| + B_2\alpha_2\alpha_3|e_{yz}|$$



[011] substrate





Conclusion

- Magnetoelastic effect provides a phenomenological way to study strain-induced magnetocrystalline anisotropy.
- It also predicts the in-plane anisotropy of [111] films