Spin-lattice models in cubic symmetry - multiscale bridge in magnetic properties

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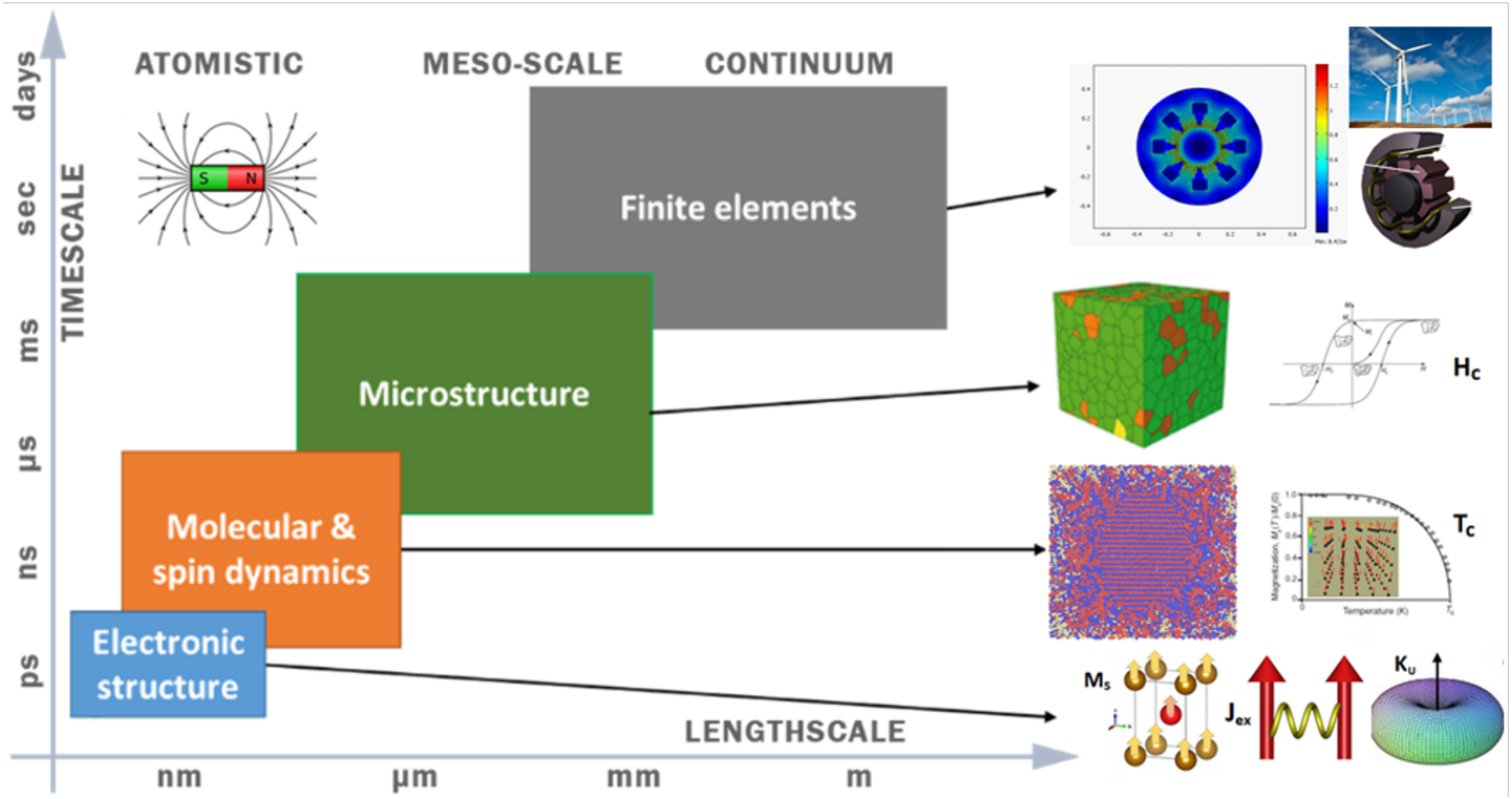








Multiscale modelling



Outline

Motivation

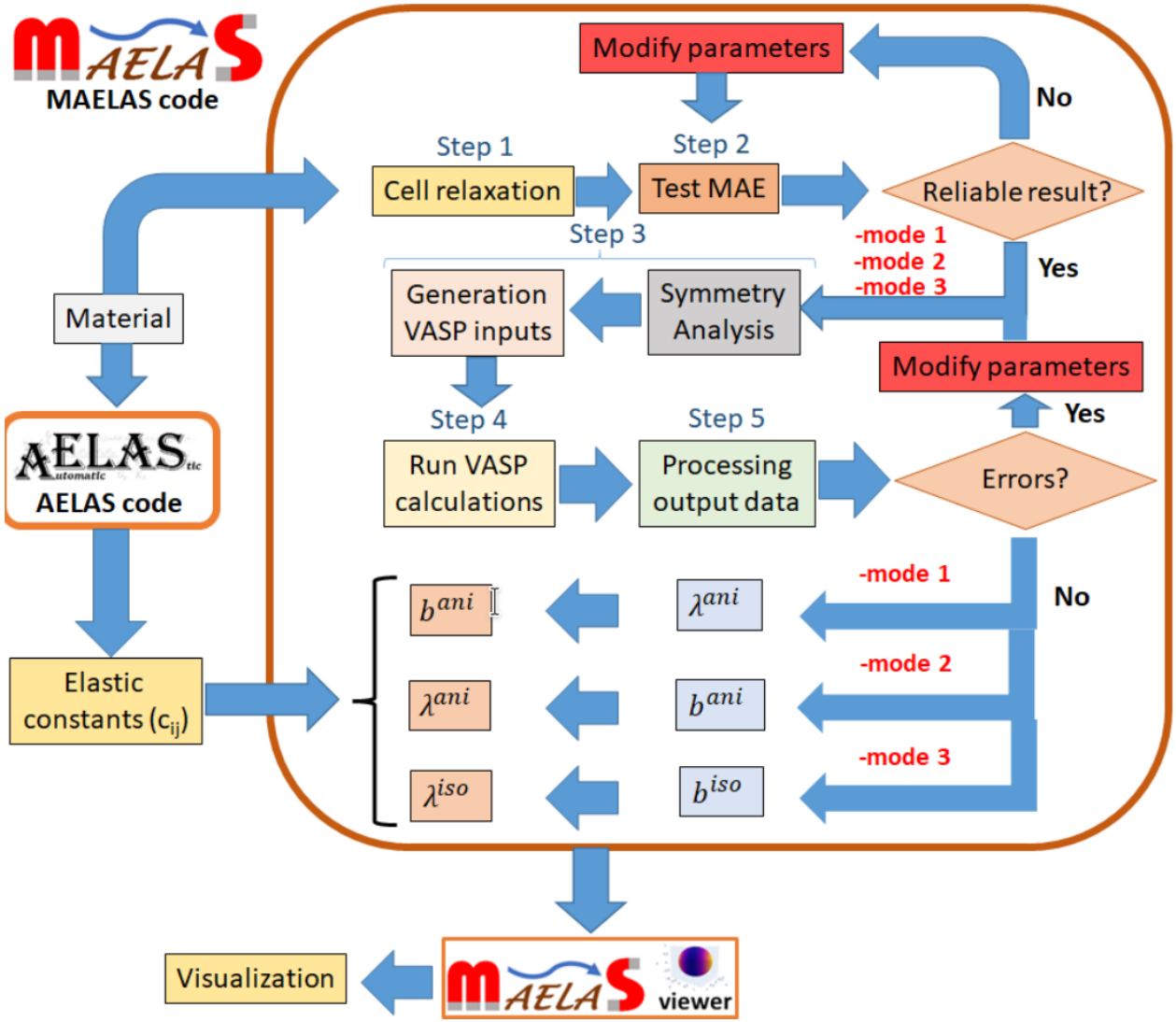
- Simulation with millions of atoms up to timescale of microseconds - to bridge the length and time scales
- Multiscale modeling of magnetic materials

Content of the talk

- Combining electronic, atomistic and magnetic degrees of freedom
- Magnetostriction & Magneto-elasticity as the central quantities for us - how do we get it from DFT...
- Why spin-lattice(SL) models in the first place?
  - SL for ferromagnetic systems (*e.g.* bcc Fe, fcc Ni)
  - SL for antiferromagnetic systems - prototype of NiO
- This leads to field of developing potentials...
- Temperature effects... not to be frozen by DFT T=0K results
- Outlook

MAELAS - general scheme - mode 1, 2 and 3

General derivation (mode 1) based on R. Wu, A. J. Freeman, J. of Appl. Phys., 79, 6209–6212 (1996).



Elastic and Magnetoelastic contributions to energy

Cubic (I)

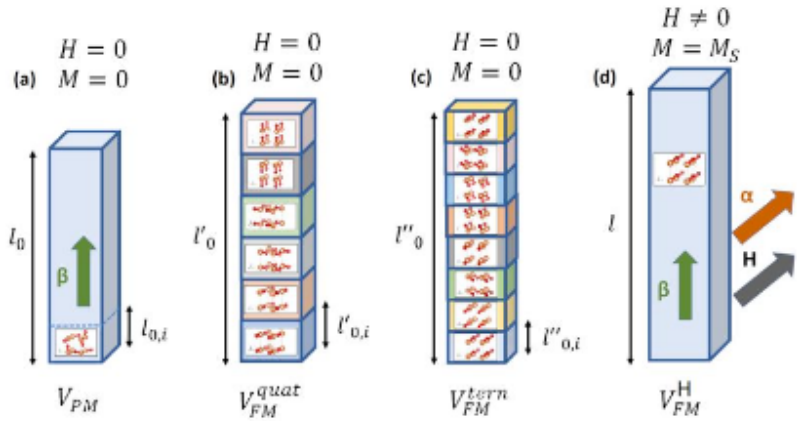
Elastic energy

$$\frac{E_{el}^{cub}-E_0}{V_0} = \frac{C_{11}}{2}(\tilde{\varepsilon}_1^2+\tilde{\varepsilon}_2^2+\tilde{\varepsilon}_3^2)+C_{12}(\tilde{\varepsilon}_1\tilde{\varepsilon}_2+\tilde{\varepsilon}_1\tilde{\varepsilon}_3+\tilde{\varepsilon}_2\tilde{\varepsilon}_3) + \frac{C_{44}}{2}(\tilde{\varepsilon}_4^2+\tilde{\varepsilon}_5^2+\tilde{\varepsilon}_6^2) = \frac{c_{xxxx}}{2}(\varepsilon_{xx}^2+\varepsilon_{yy}^2+\varepsilon_{zz}^2)+c_{xxyy}(\varepsilon_{xx}\varepsilon_{yy}+\varepsilon_{xx}\varepsilon_{zz}+\varepsilon_{yy}\varepsilon_{zz}) + 2c_{yzyz}(\varepsilon_{xy}^2+\varepsilon_{yz}^2+\varepsilon_{xz}^2),$$

Magnetoelastic energy

$$\frac{E_{me}^{cub(I)}}{V_0} = b_0(\tilde{\varepsilon}_1+\tilde{\varepsilon}_2+\tilde{\varepsilon}_3)+b_1(\alpha_x^2\tilde{\varepsilon}_1+\alpha_y^2\tilde{\varepsilon}_2+\alpha_z^2\tilde{\varepsilon}_3) + b_2(\alpha_x\alpha_y\tilde{\varepsilon}_6+\alpha_x\alpha_z\tilde{\varepsilon}_5+\alpha_y\alpha_z\tilde{\varepsilon}_4) = b_0(\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz})+b_1(\alpha_x^2\varepsilon_{xx}+\alpha_y^2\varepsilon_{yy}+\alpha_z^2\varepsilon_{zz}) + 2b_2(\alpha_x\alpha_y\varepsilon_{xy}+\alpha_x\alpha_z\varepsilon_{xz}+\alpha_y\alpha_z\varepsilon_{yz}),$$

$$\frac{\partial(E_{el}+E_{me})}{\partial\varepsilon_{ij}} = 0 \Rightarrow \varepsilon_{ij}^{eq}(\boldsymbol{\alpha}) \Rightarrow \left.\frac{\Delta l}{l_0}\right|_{\boldsymbol{\beta}}^{\boldsymbol{\alpha}} = \sum_{i,j=x,y,z}\varepsilon_{ij}^{eq}(\boldsymbol{\alpha})\beta_i\beta_j$$



$$\left.\frac{\Delta l}{l_0}\right|_{\boldsymbol{\beta}}^{\boldsymbol{\alpha}} = \lambda^{\alpha}+\frac{3}{2}\lambda_{001}\left(\alpha_x^2\beta_x^2+\alpha_y^2\beta_y^2+\alpha_z^2\beta_z^2-\frac{1}{3}\right) + 3\lambda_{111}(\alpha_x\alpha_y\beta_x\beta_y+\alpha_y\alpha_z\beta_y\beta_z+\alpha_x\alpha_z\beta_x\beta_z)$$

$$\lambda^{\alpha} = \frac{-b_0-\frac{1}{3}b_1}{c_{11}+2c_{12}}, \quad \lambda_{001} = \frac{-2b_1}{3(c_{11}-c_{12})}, \quad \lambda_{111} = \frac{-b_2}{3c_{44}}.$$

Spin-lattice (SL) model in general - cubic symmetry

Hamiltonian

$$\mathcal{H}_{sl}(\mathbf{r},\mathbf{p},\mathbf{s}) = \sum_{i=1}^{N} \frac{|\mathbf{p}_i|^2}{2m_i} + \sum_{i,j=1}^{N} \mathcal{V}(r_{ij}) + \mathcal{H}_{mag}(\mathbf{r},\mathbf{s})$$

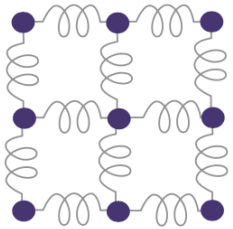
Magnetic part

$$\mathcal{H}_{mag}(\mathbf{r},\mathbf{s}) = -\frac{1}{2} \sum_{i,j=1,i\neq j}^{N} J(r_{ij})\mathbf{s}_i\mathbf{s}_j + \mathcal{H}_{Néel}(\mathbf{r},\mathbf{s}) - \mu_0 \sum_{i=1}^{N} \mu_i \mathbf{H}\mathbf{s}_i$$

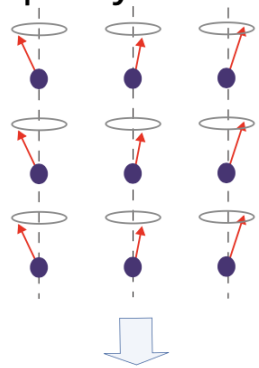
The Néel interaction

$$\begin{aligned}\mathcal{H}_{Néel} = -\frac{1}{2} \sum_{i,j=1}^{N} \{ & g(r_{ij}) + l_1(r_{ij}) \left[(\mathbf{e}_{ij}\mathbf{s}_i)(\mathbf{e}_{ij}\mathbf{s}_j) - \frac{\mathbf{s}_i\mathbf{s}_j}{3} \right] \\ & + q_1(r_{ij}) \left[(\mathbf{e}_{ij}\mathbf{s}_i)^2 - \frac{\mathbf{s}_i\mathbf{s}_j}{3} \right] \left[(\mathbf{e}_{ij}\mathbf{s}_j)^2 - \frac{\mathbf{s}_i\mathbf{s}_j}{3} \right] \\ & + q_2(r_{ij}) \left[(\mathbf{e}_{ij}\mathbf{s}_i)(\mathbf{e}_{ij}\mathbf{s}_j)^3 + (\mathbf{e}_{ij}\mathbf{s}_j)(\mathbf{e}_{ij}\mathbf{s}_i)^3 \right] \}\end{aligned}$$

Lattice dynamics



Spin dynamics



Spatial dependence of magnetic parameters

where

$$\begin{aligned}\mathbf{e}_{ij} &= \mathbf{r}_{ij}/r_{ij} \\ l_1(r_{ij}) &= l(r_{ij}) + \frac{12}{35} q(r_{ij}), \\ q_1(r_{ij}) &= \frac{9}{5} q(r_{ij}), \\ q_2(r_{ij}) &= -\frac{2}{5} q(r_{ij}).\end{aligned}$$

Spatial dependence of magnetic parameters in SL model

$$\mathcal{H}_{mag} = -\frac{1}{2}\sum_{i,j=1,i\neq j}^{N} J(r_{ij})\mathbf{s}_i\mathbf{s}_j - \frac{1}{2}\sum_{i,j=1}^{N}\{g(r_{ij}) + l_1(r_{ij})\left[(\mathbf{e}_{ij}\mathbf{s}_i)(\mathbf{e}_{ij}\mathbf{s}_j) - \frac{\mathbf{s}_i\mathbf{s}_j}{3}\right]$$
$$+ q_1(r_{ij})\left[(\mathbf{e}_{ij}\mathbf{s}_i)^2 - \frac{\mathbf{s}_i\mathbf{s}_j}{3}\right]\left[(\mathbf{e}_{ij}\mathbf{s}_j)^2 - \frac{\mathbf{s}_i\mathbf{s}_j}{3}\right] + q_2(r_{ij})\left[(\mathbf{e}_{ij}\mathbf{s}_i)(\mathbf{e}_{ij}\mathbf{s}_j)^3 + (\mathbf{e}_{ij}\mathbf{s}_j)(\mathbf{e}_{ij}\mathbf{s}_i)^3\right]\}$$

$J(r_{ij})$ — exchange parameter
(*responsible for the correct characteristic Curie or Néel temperature and the spontaneous volume magnetostriction*)

$l(r_{ij})$ — dipole term
(*describe the anisotropic effects induced by spin-orbit coupling like the anisotropic magnetostriction*)

$q(r_{ij})$ — quadrupole term
(*describe magnetocrystalline anisotropy*)

$g(r_{ij})$ — term used for shift ground state energy of the exchange interaction

The spatial dependences of $J(r_{ij})$, and $l(r_{ij})$ and $q(r_{ij})$ are described using the Bethe-Slater curve $\Lambda(r_{ij})$, as implemented in the SPIN package of LAMMPS

$$\Lambda(r_{ij}) = 4\alpha_\Lambda\left(\frac{r_{ij}}{\delta_\Lambda}\right)^2\left[1-\gamma_\Lambda\left(\frac{r_{ij}}{\delta_\Lambda}\right)^2\right]e^{-\left(\frac{r_{ij}}{\delta_\Lambda}\right)^2}\Theta(R_{c,\Lambda}-r_{ij})$$

where $\Theta(R_{c,\Lambda} - r_{ij})$ is the Heaviside step function and the $R_{c,\Lambda}$ ($\Lambda = J, l, q$) are the cut-off radii

The idea of the approach is to determine the parameters α_Λ, γ_Λ, δ_Λ($\Lambda = J, l, q$) in such a way that $J(r_{ij})$, $l(r_{ij})$, $q(r_{ij})$ **reproduce the correct magnetic properties of crystal**

[1]J. Tranchida et al. J. Comp. Phys. **372** 406 (2018)

SL for ferromagnetic cubic materials

$$\mathcal{H}_{\text{Néel}} = -\frac{1}{2}\sum_{i,j=1,i\neq j}^{N}\left\{g(r_{ij}) + l(r_{ij})\left(\cos^2\psi_{ij} - \frac{1}{3}\right) + q(r_{ij})\left(\cos^4\psi_{ij} - \frac{6}{7}\cos^2\psi_{ij} + \frac{3}{35}\right)\right\}, \cos\psi_{ij} = \boldsymbol{e}_{ij}\cdot\boldsymbol{s}_i.$$

MCA:

$$\text{SC}: q(r_0) = \frac{V_0 K_1(r_0)}{2N} = \frac{1}{2}r_0^3 K_1(r_0),$$
$$\text{BCC}: q(r_0) = -\frac{9V_0 K_1(r_0)}{16N} = -\frac{\sqrt{3}}{4}r_0^3 K_1(r_0),$$
$$\text{FCC}: q(r_0) = -\frac{V_0 K_1(r_0)}{N} = -\frac{1}{\sqrt{2}}r_0^3 K_1(r_0),$$

Bethe-Slater parameters in terms K_1 and $\frac{\delta K_1}{\delta P}$

$$\text{SC}: r_0\frac{\partial q}{\partial r}\Big|_{r=r_0} = \frac{3}{2}r_0^3 K_1(r_0)\left[1 - \frac{B}{K_1}\frac{\partial K_1}{\partial P}\right]_{r=r_0},$$
$$\text{BCC}: r_0\frac{\partial q}{\partial r}\Big|_{r=r_0} = -\frac{3\sqrt{3}}{4}r_0^3 K_1(r_0)\left[1 - \frac{B}{K_1}\frac{\partial K_1}{\partial P}\right]_{r=r_0},$$
$$\text{FCC}: r_0\frac{\partial q}{\partial r}\Big|_{r=r_0} = -\frac{3}{\sqrt{2}}r_0^3 K_1(r_0)\left[1 - \frac{B}{K_1}\frac{\partial K_1}{\partial P}\right]_{r=r_0},$$

$$\delta_q = r_0,$$
$$\alpha_q = \frac{e}{8}\left[2q(r_0) - r_0\frac{\partial q}{\partial r}\Big|_{r=r_0}\right],$$
$$\gamma_q = \frac{r_0\frac{\partial q}{\partial r}\big|_{r=r_0}}{r_0\frac{\partial q}{\partial r}\big|_{r=r_0} - 2q(r_0)}.$$

Magnetoelasticity:

$$\text{SC}: l(r_0) = -\frac{V_0 b_2}{2N}, \quad r_0\frac{\partial l}{\partial r}\Big|_{r=r_0} = -\frac{V_0 b_1}{N},$$
$$\text{BCC}: l(r_0) = -\frac{3V_0 b_1}{8N}, \quad r_0\frac{\partial l}{\partial r}\Big|_{r=r_0} = \frac{3V_0}{8N}(b_1 - 3b_2),$$
$$\text{FCC}: l(r_0) = \frac{V_0}{2N}\left(\frac{b_2}{2} - b_1\right), \quad r_0\frac{\partial l}{\partial r}\Big|_{r=r_0} = \frac{V_0}{N}\left(b_1 - \frac{3b_2}{2}\right).$$

Bethe-Slater parameters in terms of b_1 and b_2

$$\delta_l = r_0,$$
$$\alpha_l = \frac{e}{8}\left[2l(r_0) - r_0\frac{\partial l}{\partial r}\Big|_{r=r_0}\right],$$
$$\gamma_l = \frac{r_0\frac{\partial l}{\partial r}\big|_{r=r_0}}{r_0\frac{\partial l}{\partial r}\big|_{r=r_0} - 2l(r_0)}.$$

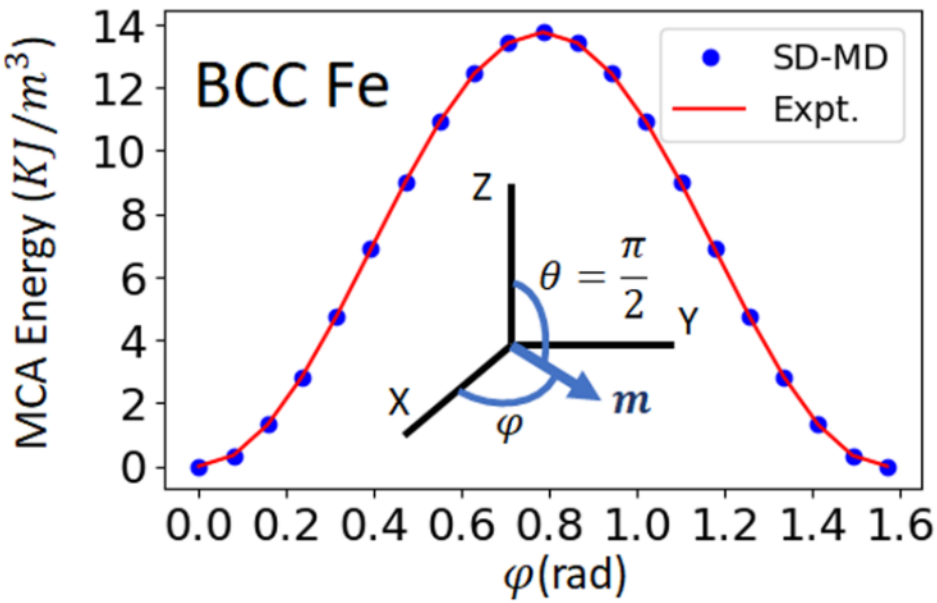
Exchange interaction:

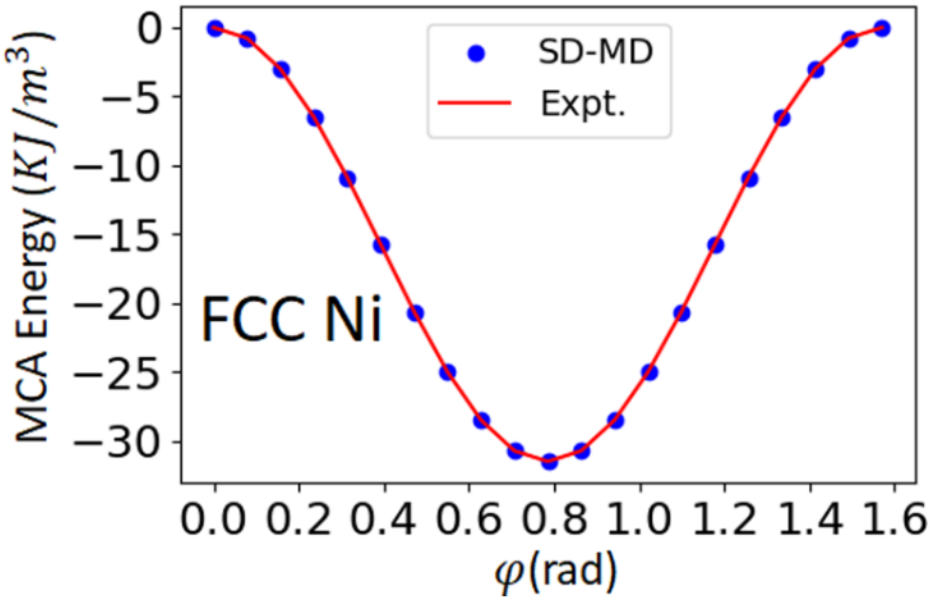
$$\text{SC}: J(r_0) = \frac{k_B T_C}{2}, \quad r_0\frac{\partial J}{\partial r}\Big|_{r=r_0} = \frac{\omega_s(c_{11}+2c_{12})V_0}{3N},$$
$$\text{BCC}: J(r_0) = \frac{3k_B T_C}{8}, \quad r_0\frac{\partial J}{\partial r}\Big|_{r=r_0} = \frac{\omega_s(c_{11}+2c_{12})V_0}{4N},$$
$$\text{FCC}: J(r_0) = \frac{k_B T_C}{4}, \quad r_0\frac{\partial J}{\partial r}\Big|_{r=r_0} = \frac{\omega_s(c_{11}+2c_{12})V_0}{6N},$$

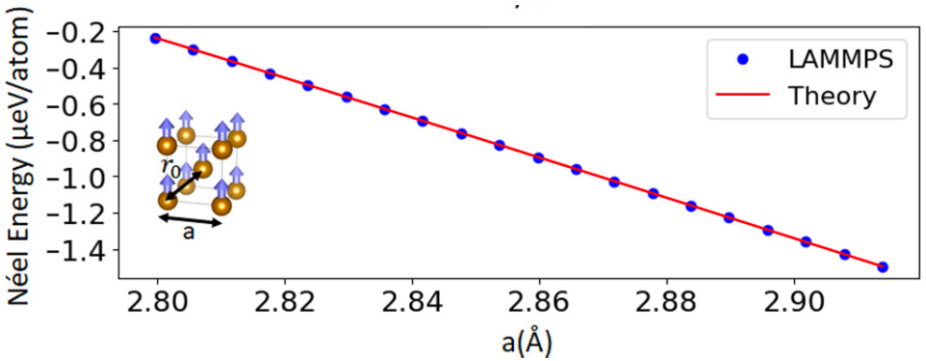
Bethe-Slater parameters in terms of ω_s

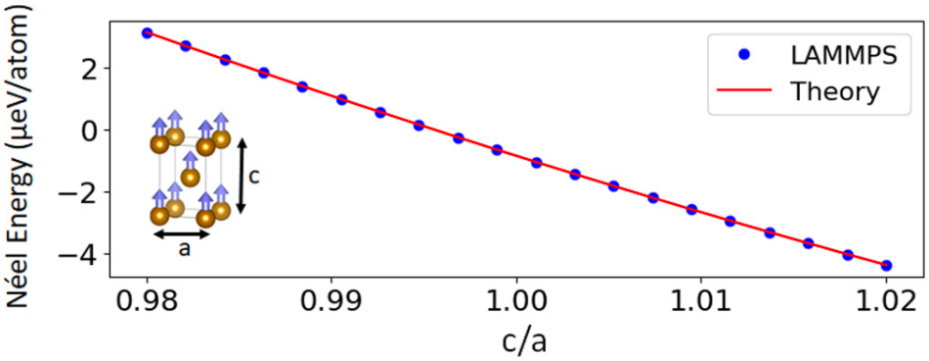
$$\delta_J = r_0,$$
$$\alpha_J = \frac{e}{8}\left[2J(r_0) - r_0\frac{\partial J}{\partial r}\Big|_{r=r_0}\right],$$
$$\gamma_J = \frac{r_0\frac{\partial J}{\partial r}\big|_{r=r_0}}{r_0\frac{\partial J}{\partial r}\big|_{r=r_0} - 2J(r_0)},$$

SL for FM cubic materials - Néel energy and MCA







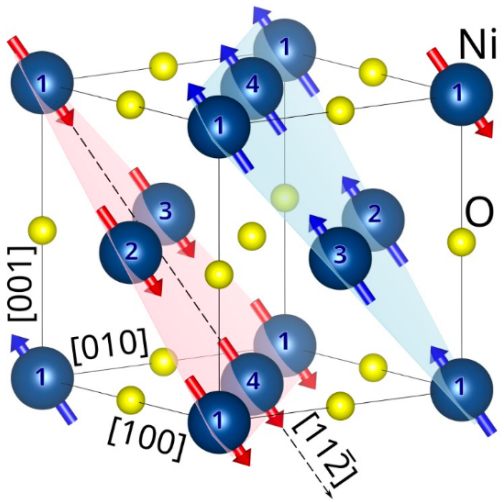


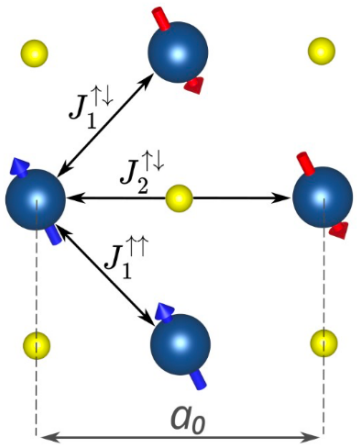
Results: for FM BCC Fe and FCC Ni

Material	Elastic constants	SD-MD (GPa)	Expt. (GPa)	Magnetostrictive coefficients	SD-MD ($\times 10^{-6}$)	Expt. ($\times 10^{-6}$)
BCC Fe	c_{11}	230.0	230[a]	λ_{001}	25.9	26[c]
	c_{12}	134.1	135[a]	λ_{111}	−30.3	−30[c]
	c_{44}	116.3	117[a]			
FCC Ni	c_{11}	263.9	261.2[b]	λ_{001}	−61.9	−60[c]
	c_{12}	152.1	150.8[b]	λ_{111}	−35.4	−35[c]
	c_{44}	132.8	131.7[b]			

Material	MCA	SD-MD (KJ/m^3)	Expt. (KJ/m^3)	MCA vs P	SD-MD (GPa^{-1})	Expt. (GPa^{-1})
BCC Fe	K_1	54.995	55[d]	$\frac{1}{K_1}\frac{\partial K_1}{\partial P}$	−0.0727	−0.073[e]
FCC Ni	K_1	−125.996	−126[d]	$\frac{1}{K_1}\frac{\partial K_1}{\partial P}$	−0.0279	−0.028[e]

SL for antiferromagnetic cubic materials - case of NiO





Bethe-Slater curve

$$\Lambda(r_{ij}) = 4\alpha_\Lambda \left(\frac{r_{ij}}{\delta_\Lambda}\right)^2 \left[1 - \gamma_\Lambda \left(\frac{r_{ij}}{\delta_\Lambda}\right)^2\right] e^{-\left(\frac{r_{ij}}{\delta_\Lambda}\right)^2} \Theta(R_{c,\Lambda} - r_{ij})$$

$$\delta_\Lambda = r_0$$

$$\alpha_\Lambda = \frac{e}{8}\left[2\Lambda(r_0) - r_0 \frac{\partial \Lambda}{\partial r}\Big|_{r=r_0}\right] \qquad (\Lambda = J, I, q)$$

$$\gamma_\Lambda = \frac{r_0 \frac{\partial \Lambda}{\partial r}\Big|_{r=r_0}}{r_0 \frac{\partial \Lambda}{\partial r}\Big|_{r=r_0} - 2\Lambda(r_0)}$$

Different types of neighbors require different parameterizations of $J(r_{ij})$, $I(r_{ij})$ and $q(r_{ij})$ terms

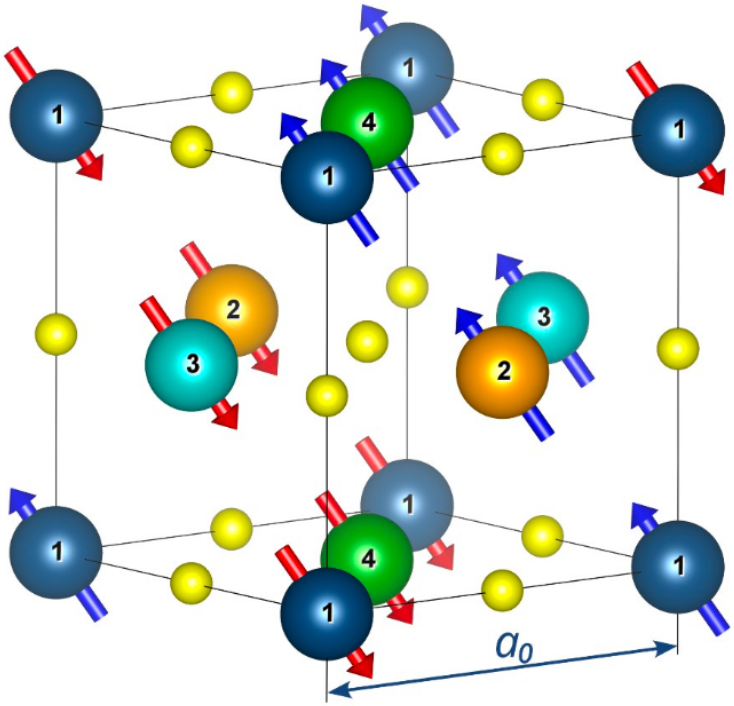
$(\mathbf{s_i}.\mathbf{s_j} = 1)$

$$\mathcal{H}^{\uparrow\uparrow}_{N\acute{e}el}(\mathbf{r},\mathbf{s}) = -\frac{1}{2}\sum_{i,j=1,i\neq j}^{N}\{g(r_{ij}) + l(r_{ij})\left[(\mathbf{e}_{ij}\mathbf{s}_i)^2 - \frac{1}{3}\right] + q(r_{ij})\left[(\mathbf{e}_{ij}\mathbf{s}_i)^4 - \frac{6}{7}(\mathbf{e}_{ij}\mathbf{s}_i)^2 + \frac{3}{35}\right]\}$$

$(\mathbf{s_i}.\mathbf{s_j} = -1)$

$$\mathcal{H}^{\uparrow\downarrow}_{N\acute{e}el}(\mathbf{r},\mathbf{s}) = -\frac{1}{2}\sum_{i,j=1,i\neq j}^{N}\{g(r_{ij}) - l(r_{ij})\left[(\mathbf{e}_{ij}\mathbf{s}_i)^2 - \frac{1}{3}\right] + q(r_{ij})\left[\frac{13}{5}(\mathbf{e}_{ij}\mathbf{s}_i)^4 + \frac{6}{7}(\mathbf{e}_{ij}\mathbf{s}_i)^2 + \frac{11}{35}\right]\}$$

SL: Cubic antiferromagnetic - case of NiO



Definition of the simple cubic (SC) Ni^{2+} sublattices in NiO. Each of the 4 SC sublattices, in turn, consists of two sublattices with spin up and spin down

$J_2^{\uparrow\downarrow} \gg J_1^{\uparrow\uparrow}, J_1^{\uparrow\downarrow}$ ⟹ only NNNs are considered

SC AFM:

$$J(r_0) = -\frac{k_B T_N}{2},\ r_0 \frac{\partial J}{\partial r}\Big|_{r=r_0} = -\frac{\omega_s (C_{11} + 2C_{12}) V_0}{3n}$$

$$l(r_0) = \frac{V_0 b_2}{2n},\ r_0 \frac{\partial l}{\partial r}\Big|_{r=r_0} = \frac{V_0 b_1}{n}$$

$$q(r_0) = \frac{5 V_0 K_1}{26n},\ r_0 \frac{\partial q}{\partial r}\Big|_{r=r_0} = \frac{15 V_0 K_1}{26n}\left[1 - \frac{B}{K_1}\frac{\partial K_1}{\partial P}\right]$$

$V_0 = a_0^3$ is the volume of the unit cell of NiO, n = 4 is number of the magnetic interacting atoms in V_0 that have been included in the model.

SL model parameters α_Λ, γ_Λ, δ_Λ (Λ = J, l, q) for NiO

SD-MD parameters	SD-MD 1	SD-MD 2
$R_{c,J}$ (Å)	4.5	4.5
α_J (meV/atom)	-26.97232	-27.07260
γ_J	0.4322455	0.4343486
δ_J (Å)	4.18969	4.25129
$R_{c,l}$ (Å)	4.5	4.5
α_l (μeV/atom)	29.15117	30.45598
γ_l	-1.502436	-1.502436
δ_l (Å)	4.18969	4.25129
$R_{c,q}$ (Å)	4.5	4.5
α_q (μeV/atom)	3.812218	3.814495
γ_q	0.5459437	0.5259032
δ_q (Å)	4.18969	4.25129

SD-MD 1 - interionic Born potential model of ionic solids

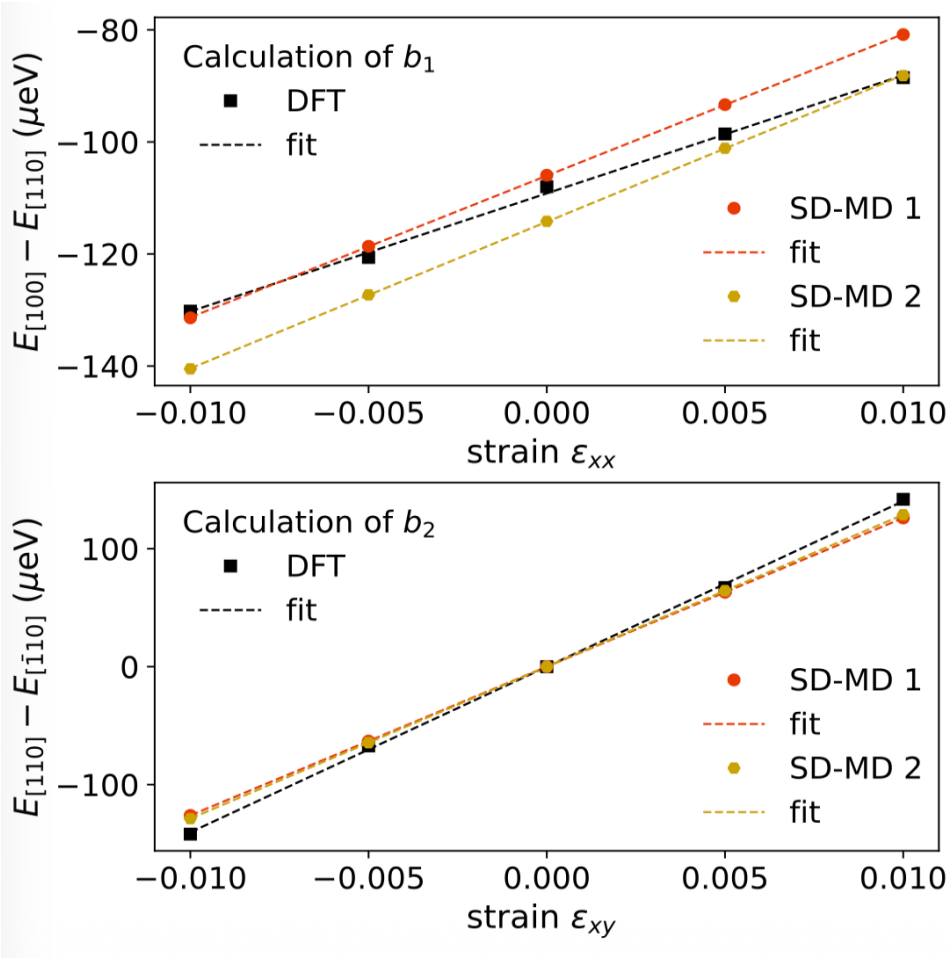
SD-MD 2 - RF-MEAM potential that we parametrized to C_{ij}.

$$\phi(r_{ij}) = A\exp(-Br_{ij}) - \frac{C}{r_{ij}^6}$$

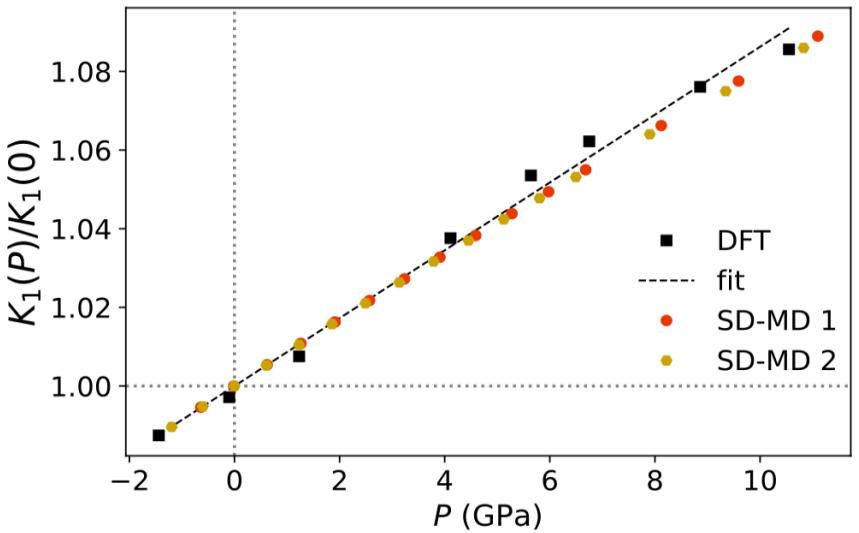
Interaction	A (eV)	B (Å^{-1})	C (eV Å^6)
$Ni^{2+} - Ni^{2+}$	0	1	0
$Ni^{2+} - O^{2-}$	754.92	3.05157	0
$O^{2-} - O^{2-}$	22764.3	6.71141	27.89

[1] C. A. J. Fisher, H. Matsubara, Philosophical Magazine **85**, 1067–1088 (2005).

Results of SL(SD-MD) for AF cubic NiO



- Magnetoelastic constants b_1 and b_2 through a linear fitting of the energy versus strain data. Comparison of the results obtained with DFT and SD-MD.
- The hydrostatic pressure (P) effect on MCA (K_1)

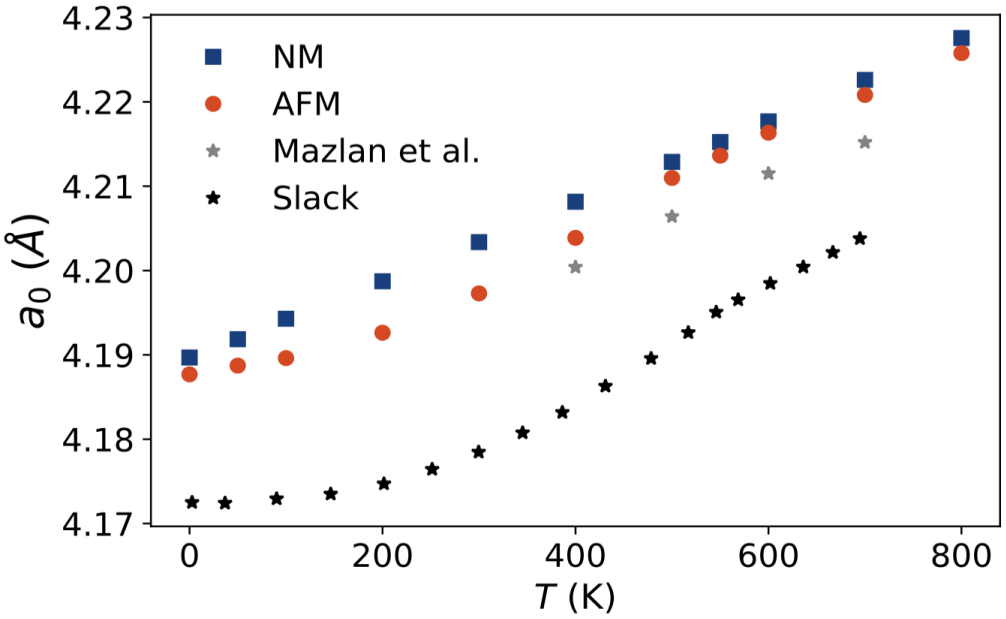


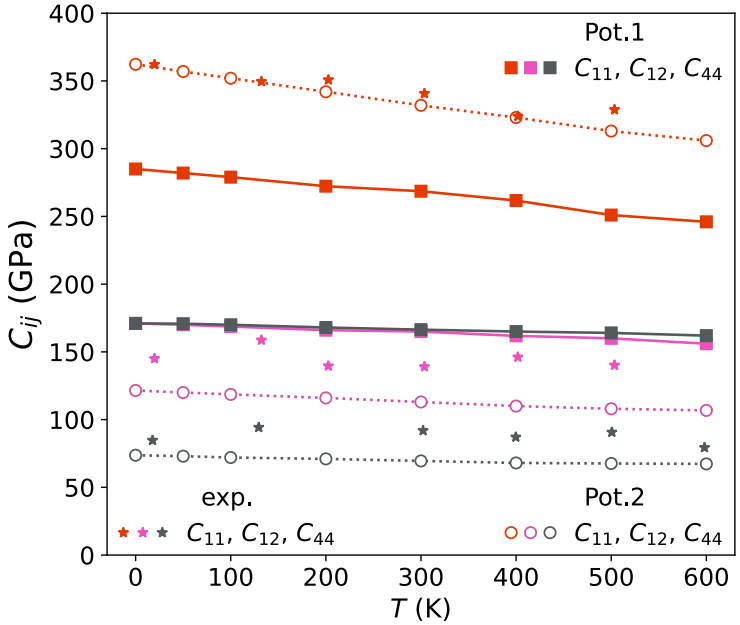
Results of SL(SD-MD) for AF NiO...

Parameters	SD-MD 1	SD-MD 2	Calc. (present work)	Calc.	Expt.
a_0^{NM} (Å)	4.18969	4.25129			
a_0^{AFM} (Å)	4.18769	4.24927	4.20	4.190[25]	4.1705[41]
a_0^{PM} (Å)	4.18969	4.25125		4.192[25]	
$J_2^{\uparrow\downarrow}$ (meV)	-22.5	-22.5		-14.0[50]	-19.04[41]
$J_1^{\uparrow\uparrow}$, $J_1^{\uparrow\downarrow}$ (meV)	0	0		1.2, -1.2[50]	1.39, -1.35[41]
ω_s	-0.00143	-0.00140		-0.00143[25]	
C_{11} (GPa)	285	362	358	274[31]	358[44]
C_{12} (GPa)	171	121	109	170[31]	134[44]
C_{44} (GPa)	171	74	86	83[31]	93[44]
B (GPa)	209	202	192	194[25]	180 – 220[51]
b_1 (MPa)	1.38	1.42	1.12		
b_2 (MPa)	1.72	1.75	1.87		
λ_{100} ($\times 10^{-4}$)	-0.080	-0.039	-0.030	-1.45[47]	
λ_{111} ($\times 10^{-4}$)	-0.033	-0.079	-0.072	-0.79[47]	
K_1 (kJ m^{-3})	115.42	115.42	115.42	113.5[49]	
$\frac{1}{K_1}\frac{\partial K_1}{\partial P}$ (GPa^{-1})	0.00816	0.00811	0.00862		

Temperature depedent results of SD-MD for AF NiO

- Temperature dependence of the lattice constant a_0 obtained from the interionic potential modeled by Fisher and Matsubara only (NM) and with added magnetic part (SL) for the AFM ordering, NVT simulations.





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Conclusion

- Bridge the length scales from DFT to atomistic simulations - **SL models**
- Very good agreement on MAE, magneto-elastic ($b's$), magnetostrictive properties ($\lambda's$) between DFT and atomistic simulations
- Obtaining one potential describing PM and FM/AFM behavior

Published at:

- **SL model for FM bcc Fe, fcc Ni** P. Nieves, J. Tranchida, S. Arapan, D. Legut, Phys. Rev **B** 103 094437 (2021)
- **SL model for AFM NiO** I. Korrnienko, P. Nieves, J. Šebesta, R. Iglesias, D. Legut, J. Chem. Phys. **165**, 024701 (2026)
- **SL model for AFM FeRh**, taken into account FM and AFM interactions, S. Arapan, K. Padrón-Alemán, I. Korniienko, R. Iglesias, P. Álvarez-Alonso, J. A. Blanco, P. Gorria, and D. Legut, Comm. Phys., https://doi.org/10.1038/s42005-026-02758-6)

Current usage of SL models:

- Atomistic simulations of magnetoelastic effects on sound velocity, P. Nieves, J. Tranchida, S. Nikolov, A. Fraile, D. Legut, Phys. Rev B **105**, 134430 (2022)
- Computational study of elastic waves generated by ultrafast demagnetization in fcc Ni, I. Korniienko, P. Nieves, A. Fraile, R. Iglesias, D. Legut, Phyd. Rev. Res. **6**, 023311 (2024).
- Simon effect (speed of sound under magnetic field) in cubic FM materials, I. Korniienko, D. Legut, et al., Res. in Phys **73**, 108264 (2025)
- The effect of the magnon–phonon resonance on the sound wave propagation in bcc Fe, I. Kornienko, P. Nieves, D. Legut (JMMM - accepted)

Relation between various notations of magnetostriction

Clark

Hexagonal system

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Gauge direction β_x β_y β_z	Magnetization direction Initial α_x α_y α_z	Final α_x α_y α_z	$\lambda(x,y)_0-\lambda(x,y)_f$	Magnetostriction coefficients Eq. (3)	Mason[a]	Birss[b]
1 0 0	1 0 0	0 1 0	$\lambda(a,a)-\lambda(b,a)$	$\lambda^{\gamma,2}$	$\lambda_A-\lambda_B$	Q_3
0 0 1	0 0 1	1 0 0	$\lambda(c,c)-\lambda(a,c)$	$\lambda_2^{\alpha,2}$	$-\lambda_C$	$-Q_2-Q_4$
1 0 0	1 0 0	0 1 0	$\lambda(a,a)-\lambda(c,a)$	$-\lambda_1^{\alpha,2}+\frac{1}{2}\lambda^{\gamma,2}$	λ_A	$-Q_2$
$\frac{\sqrt{2}}{2}$ 0 $\frac{\sqrt{2}}{2}$	$\frac{\sqrt{2}}{2}$ 0 $\frac{\sqrt{2}}{2}$	$\frac{\sqrt{2}}{2}$ 0 $\frac{\sqrt{2}}{2}$	$\lambda(d,d)-\lambda(e,d)$	$\lambda^{\epsilon,2}$	$-\frac{1}{2}\lambda_A-\frac{1}{2}\lambda_C+2\lambda_D$	$\frac{1}{2}Q_6$

[a] W. P. Mason, Phys. Rev. 96, 302 (1954).
[b] R. R. Birss, *Advances in Physics* (Francis & Taylor, Ltd., London, 1959), Vol. 8, p. 252.

MAELAS notation

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Callen

$$\lambda_{11}^{\alpha}=2\lambda_1^{\alpha,0}+\lambda_2^{\alpha,0}+2\lambda_1^{\alpha,2}+$$
$$(\sqrt{3}/2)\lambda_{12}^{\alpha}=2\lambda_1^{\alpha,2}+\lambda_2^{\alpha,2},$$
$$2\lambda_{21}^{\alpha}=-\lambda_1^{\alpha,0}+\lambda_2^{\alpha,0},$$
$$\sqrt{3}\lambda_{22}^{\alpha}=-\lambda_1^{\alpha,2}+\lambda_2^{\alpha,2}.$$
$$\lambda^{\epsilon}=\lambda^{\epsilon,2}$$
$$\lambda^{\gamma}=\lambda^{\gamma,2}$$

The calculated magnetostrictive coefficients are written in Clark, Mason, Birss and Callen notation in MAELAS code