Spin-lattice model for cubic crystals

P. Nieves, J. Tranchida, S. Arapan, and D. Legut

1 IT4Innovations, VSB - Technical University of Ostrava, 17. listopadu 2172/15, 70800 Ostrava-Poruba, Czech Republic and
2 Computational Multiscale Department, Sandia National Laboratories, P.O. Box 5800, MS 1322, 87185 Albuquerque, NM, United States

(Dated: December 11, 2020)

We present a methodology based on the Néel model to build spin-lattice models for cubic crystals capable of describing magnetic properties induced by the spin-orbit coupling like magnetoelastic anisotropy and anisotropic magnetostriction. The dipole and quadrupole terms of the Néel model are parameterized through the Bethe-Slater curve. We apply this method to develop a spin-lattice model for BCC Fe and FCC Ni, and we show that it accurately reproduces the experimental elastic tensor, magnetocrystalline anisotropy under pressure, and anisotropic magnetostrictive coefficients at zero-temperature. This work could constitute a step towards large-scale modeling of magnetoelastic phenomena.

PACS numbers: 31.15.A-, 75.50.Ww, 75.30.Gw, 07.05.Tp

I. INTRODUCTION

Magnetoelastic interactions couple the motion of atoms in a magnetic material with atomic magnetic moments, and allow to transfer mechanical and thermal energies between phonon and magnon subsystems.[4] Magnetoelasticity is of great interest for applications, but also from a fundamental point of view. For instance, precise control of magnetization through a mechanical excitation of the motion of atoms in magnetic materials, and vice versa, has enabled the development of a wide range of technological applications such as sensors (torque sensors, motion and position sensors, force and stress sensors) and actuators (sonar transducer, linear motors, rotational motors, and hybrid magnetostrictive/piezoelectric devices).[21] Similarly, the combination of magnetism and heat is exploited in many applications like heat-assisted magnetic recording (HAMR),[9] thermally assisted magnetic random access memory (MRAMs),[7] ultrafast all-optically induced magnetization dynamics,[8] magnetic refrigeration,[10] and biomedical magnetic hyperthermia.[11]

Magnetoelastic effects can also have a strong influence on the thermo-mechanical properties of materials. This is for example the case of the phononic component of the thermal conductivity. Though magnon-phonon scattering can abruptly change through magnetic phase-transitions,[21] for metallic oxides presenting strong magnetoelastic effects, and for which accurate thermal conductivity predictions can be of practical importance (such as uranium dioxide[12]), the development of accurate numerical models is still an ongoing process.

Presently, the theoretical and modeling techniques have reached a great level of development and accuracy to describe the uncoupled dynamics of magnons and phonons at different spatial and time scales. Typically, in magnetic materials this is done by constraining or neglecting either the motion of atomic magnetic moments or atoms. For example, in spin-polarized ab-initio molecular dynamics (AIMD) magnetic moments are constrained in certain directions and only atomic positions are updated in each time step, while in classical atomistic spin dynamics (SD) and molecular dynamics (MD) the motion of atoms or spins are neglected, respectively.[13,17] However, it is still a challenge to find suitable modeling approaches to deal with processes where the interaction between magnons and phonons is essential, like in magneto-caloric and magneto-elastic phenomena. The lack of such models is limiting the multi-scale design of materials suitable for relevant technological applications based on these physical processes. Recently, novel attempts to address this problem have been proposed. Stockem et al. demonstrated that for small supercells, a consistent interface can be designed to couple spin-polarized AIMD and classical SD.[27] Although offering an excellent level of accuracy, this approach presents the space and time scale limitations of first-principles approaches, and does not appear to be suited for running meso-scale magneto-elastic simulations. Another concept, referred to as “spin-lattice dynamics”, is based on the combination of classical spin and molecular dynamics (SD-MD), which includes the spatial dependence of exchange integrals in the spin equation of motion, among other features.[19,25] The computational cost of this classical approach scales linearly with the number of magnetic atoms in the system.[25] Combined to accurate massively parallel algorithms, this enables the simulation of multi-million magnetic atom systems on time scales sufficient to accurately study magnon-phonon relaxation processes.[21,25]

These new ideas have opened up interesting opportunities and questions about how to model and study magneto-caloric and magneto-elastic phenomena within a multi-scale approach. In particular, the coarse-grained modeling of spin-orbit coupling (SOC) through magnetocrystalline anisotropy (MCA) in SD-MD is currently a bottleneck of this issue.[25] The single-ion model of MCA is widely used in SD, but unfortunately it does not couple atom and spin degrees of freedom. This drawback can be overcome using the Néel model (two-ion model) that reproduces the correct symmetry of MCA, and couples atom and spin motion. Hence, despite some limitations of the Néel model concerning non-magnetic atoms and its phenomenological nature,[22] it seems a promising starting point to build a SD-MD model capable of simulating magneto-caloric and magneto-elastic phenomena. In this work, we propose a general procedure to find the parameters of the Néel model within the Bethe-Slater curve[22,28] that re-
produces the MCA and anisotropic magnetoelastic properties for cubic crystals at zero-temperature accurately.

II. METHODOLOGY

A. Spin-Lattice Hamiltonian

In the following discussion, we consider the spin-lattice Hamiltonian

\[
\mathcal{H}_L (\mathbf{r}, \mathbf{p}, \mathbf{s}) = \mathcal{H}_{mag}(\mathbf{r}, \mathbf{s}) + \sum_{i=1}^{N} \frac{p_i}{2m_i} + \sum_{i<j} V(r_{ij}),
\]

where \( \mathbf{r}_i, \mathbf{p}_i, \mathbf{s}_i, \) and \( m_i \) stand for the position, momentum, normalized magnetic moment and mass for each atom \( i \) in the system, respectively, \( V(r_{ij}) = V(|\mathbf{r}_i - \mathbf{r}_j|) \) is the interatomic potential energy and \( N \) is the total number of atoms in the system with total volume \( V \). Here, we include the following interactions in the magnetic energy

\[
\mathcal{H}_{mag}(\mathbf{r}, \mathbf{s}) = -\mu_0 \sum_{i=1}^{N} \mathbf{H} \cdot \mathbf{s}_i - \sum_{i<j=1}^{N} J(r_{ij}) (\mathbf{s}_i \cdot \mathbf{s}_j - 1) + \mathcal{H}_{Néel}(\mathbf{r}, \mathbf{s}),
\]

where \( \mu_0 \) is the atomic magnetic moment, \( \mu_0 \) is the vacuum permeability, \( \mathbf{H} \) is the external magnetic field, \( J(r_{ij}) \) is the exchange parameter. The exchange interaction is offset by subtracting the spin ground state (corresponding to a purely ferromagnetic situation), as detailed in Ma et al.\cite{ma2012} This offset of the exchange energy does not affect the precession dynamics of the spins. However, it allows to offset the corresponding mechanical forces. Without this additional term, the forces and the pressure are not zero at the energy ground state. The term \( \mathcal{H}_{Néel} \) is the Néel interaction

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

where \( \mathbf{e}_{ij} = \mathbf{r}_{ij}/r_{ij} \), and

\[
l_1(r_{ij}) = l(r_{ij}) + 12\frac{q(r_{ij})}{35}, \\
q_1(r_{ij}) = \frac{9}{2} q(r_{ij}), \\
q_2(r_{ij}) = -\frac{2}{5} q(r_{ij}).
\]

In the case of a collinear state (\( \mathbf{s}_i \parallel \mathbf{s}_j \)), the Eq.\cite{3} is reduced to

\[
\mathcal{H}_{Néel} = -\frac{1}{2} \sum_{i,j=1}^{N} \left\{ g(r_{ij}) + l_1(r_{ij}) \right\} \left( \cos^2 \psi_{ij} - \frac{1}{3} \right) \\
+ q(r_{ij}) \left( \cos^4 \psi_{ij} - \frac{6}{7} \cos^2 \psi_{ij} + \frac{3}{35} \right),
\]

where \( \psi_{ij} \) is the Néel energy reproduces the correct symmetry of MCA and magnetoelastic energy.\cite{3} The quantity \( g(r_{ij}) \) can be related to the volume magnetostriction induced by the exchange interactions, while the dipole (\( l(r_{ij}) \)) and quadrupole (\( q(r_{ij}) \)) terms can describe the effects induced by SOC like the anisotropic magnetostriction and MCA, respectively.\cite{31} In this work, we focus on the SOC induced effects, so that we don’t analyze the volume magnetostriction (\( g(r_{ij}) = 0 \)). In principle, one could apply a similar methodology as in Section II B to include \( g(r_{ij}) \) in the SD-MD model, and simulate the volume magnetostriction.\cite{31}

Here, we take into account the spatial dependence of \( J(r_{ij}) \), \( l(r_{ij}) \) and \( q(r_{ij}) \) using the Bethe-Slater curve, as implemented in the SPIN package of LAMMPS.\cite{25}

\[
J(r_{ij}) = 4\alpha J \left( \frac{r_{ij}}{\delta_j} \right)^2 \left[ 1 - \gamma J \left( \frac{r_{ij}}{\delta_j} \right)^2 e^{-\left( \frac{r_{ij}}{\delta_j} \right)^2} \right] \Theta(R_{c,J} - r_{ij}),
\]

\[
l(r_{ij}) = 4\alpha l \left( \frac{r_{ij}}{\delta_j} \right)^2 \left[ 1 - \gamma l \left( \frac{r_{ij}}{\delta_j} \right)^2 e^{-\left( \frac{r_{ij}}{\delta_j} \right)^2} \right] \Theta(R_{c,l} - r_{ij}),
\]

\[
q(r_{ij}) = 4\alpha q \left( \frac{r_{ij}}{\delta_j} \right)^2 \left[ 1 - \gamma q \left( \frac{r_{ij}}{\delta_j} \right)^2 e^{-\left( \frac{r_{ij}}{\delta_j} \right)^2} \right] \Theta(R_{c,q} - r_{ij}),
\]

where \( \Theta(R_{c,n} - r_{ij}) \) is the Heaviside step function and \( R_{c,n} \) is the cut-off radius. The parameters \( \alpha, \gamma, \delta \) must be determined in order to reproduce the Curie temperature (\( T_C \)), magnetostriction and MCA via \( J(r_{ij}) \), \( l(r_{ij}) \) and \( q(r_{ij}) \), respectively. The parameterization of \( J(r_{ij}) \) with the Bethe-Slater curve is a well established procedure. For instance, to find the values of \( \alpha, \gamma, \delta \), one can fit the Bethe-Slater curve to exchange parameters calculated at fixed equilibrium positions at zero-temperature. However, the parameterization of \( l(r_{ij}) \) and \( q(r_{ij}) \) with the Bethe-Slater curve is a quite new approach, so that it is not clear how to obtain the values of these parameters yet. In Section II B we propose a general procedure to obtain these parameters for cubic crystals. In the present work, we perform the analysis of this model only at zero-temperature. The equations of motion of this model at finite-temperature are those implemented in the SPIN package of LAMMPS.\cite{25,178} A detailed description of these equations can be found in Ref.\cite{25}

B. Procedure to calculate the Bethe-Slater parameters of Néel interaction for cubic crystals

The basic idea to calculate the Bethe-Slater parameters for the Néel interaction is to find the theoretical relations that link Eq.\cite{5} to both the MCA and magnetoelastic energies. To illustrate this method, we will apply it to simple cubic (SC), body-centered cubic (BCC) and face-centered cubic (FCC) crystals. The MCA energy for cubic systems reads\cite{32}

\[
\mathcal{H}_{MCA}^{\text{cub}}(\alpha, r) = V K_1(r) \left( \alpha_1^2 \alpha_2^2 + \alpha_2^2 \alpha_3^2 + \alpha_3^2 \alpha_1^2 \right),
\]

where \( K_1 \) is the first MCA constant with units of energy per volume, \( r \) is the distance to the first nearest neighbor, \( V \) is
the volume of the system, and \( \alpha_i (i = x, y, z) \) are the direction cosines of (magnetization). From this equation we have

\[
VK_1 (r) = 4 \left[ g_{\text{MCA}}^{\text{cub}} \left( \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0, r \right) - g_{\text{MCA}}^{\text{cub}} (1, 0, 0, r) \right].
\]  

Next, we evaluate the Eq. [5] with magnetic moment directions \( \mathbf{s} = (1, 1, 0, 0) \) and \( \mathbf{s} = (0, 0, 0, 1) \) up to first nearest neighbors, and we replace it in Eq. [8] in order to ensure that the Néel energy gives the correct MCA energy. And by doing so, we find the following relations for SC, BCC, and FCC

\[
\begin{align*}
SC : q(r_0) &= \frac{V_0 K_1 (r_0)}{2N} = \frac{1}{2} r_0^3 K_1 (r_0), \\
BCC : q(r_0) &= -\frac{9V_0 K_1 (r_0)}{16N} = -\frac{3\sqrt{3}}{4} r_0^3 K_1 (r_0), \\
FCC : q(r_0) &= -\frac{V_0 K_1 (r_0)}{N} = \frac{1}{\sqrt{2}} r_0^3 K_1 (r_0),
\end{align*}
\]

where \( r_0 \) is the equilibrium distance to the first nearest neighbors, and \( N \) is the number of atoms in the equilibrium volume \( V_0 \). Here, \( q(r_0) \) has units of energy per atom. In Appendix A, we show that the derivative of \( q(r) \) with respect to \( r \) can be written as

\[
\begin{align*}
SC : \frac{\partial q}{\partial r} \bigg|_{r = r_0} &= \frac{3}{2} r_0^2 K_1 (r_0) \left[ 1 - B \frac{\partial K_1}{\partial P} \right]_{r = r_0}, \\
BCC : \frac{\partial q}{\partial r} \bigg|_{r = r_0} &= -\frac{3\sqrt{3}}{4} r_0^2 K_1 (r_0) \left[ 1 - B \frac{\partial K_1}{\partial P} \right]_{r = r_0}, \\
FCC : \frac{\partial q}{\partial r} \bigg|_{r = r_0} &= -\frac{3}{2} r_0^2 K_1 (r_0) \left[ 1 - B \frac{\partial K_1}{\partial P} \right]_{r = r_0},
\end{align*}
\]

where \( B \) is the bulk modulus and \( P \) is pressure. Here, \( r_0 \partial q/\partial r \) has units of energy per atom. Note that the dipole term in Eq. [5] is canceled out, so that it does not contribute to the MCA in the cubic crystal symmetry. Since we are only considering Néel interactions up to the first nearest neighbors, we set the cut-off radius \( R_{c,a} \) in between the first and second nearest neighbors in Eq. \[6\] that is

\[
q(r_0) = 4\alpha q \left( \frac{r_0}{\delta q} \right)^2 \left[ 1 - \gamma_q \left( \frac{r_0}{\delta q} \right)^2 \left( \frac{\alpha^2}{\delta q} \right)^2 \right].
\]

The derivative of this function with respect to \( r \) is

\[
\frac{\partial q}{\partial r} \bigg|_{r = r_0} = \frac{8\alpha q r_0 e^{-\left( \frac{r_0}{\delta q} \right)^2}}{\delta q} \left[ \gamma_q \left( \frac{r_0}{\delta q} \right)^2 \left( \frac{\alpha^2}{\delta q} \right)^2 + \delta_q \right].
\]  

Hence, we have two equations with three unknown variables \( \alpha_q, \gamma_q, \) and \( \delta_q \). A reasonable strategy to reduce the number of unknown variables is to set \( \delta_q \) equal to the equilibrium distance to the first nearest neighbors \( r_0 (\delta_q = r_0) \) because it has unit of distance and can be easily estimated. Hence, solving Eqs. \[11\] and \[12\] gives

\[
\begin{align*}
\delta_q &= r_0, \\
\alpha_q &= e \left[ 2q(r_0) - r_0 \frac{\partial q}{\partial r} \bigg|_{r = r_0} \right], \\
\gamma_q &= \frac{r_0 \frac{\partial q}{\partial r} \bigg|_{r = r_0}}{r_0^2} - 2q(r_0).
\end{align*}
\]

These are the Bethe-Slater parameters in terms of \( K_1 \) and \( \partial K_1 / \partial P \) (via Eqs. \[9\] and \[10\]) to model the physics of MCA within the Néel model.

Let’s now find the values of the Bethe-Slater parameters that simulate magnetostriiction. The magnetoelastic energy for cubic systems (point groups 432, 43m, m3m) reads\[13,15\]

\[
g_{\text{me}}^{\text{cub}} = b_0 (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) + b_1 (\alpha_x^2 \varepsilon_{xx} + \alpha_y^2 \varepsilon_{yy} + \alpha_z^2 \varepsilon_{zz}) + b_2 (\alpha_x \alpha_y \varepsilon_{xy} + \alpha_x \alpha_z \varepsilon_{xz} + \alpha_y \alpha_z \varepsilon_{yz}),
\]

where \( b_0, b_1 \) and \( b_2 \) are the magnetoelastic constants, and \( \varepsilon_{ij} \) are the elements of the strain tensor. After evaluating the Néel energy (Eq. \[4\]) for a strained cubic crystal up to first nearest neighbors, and equalizing it to Eq. \[14\] one finds for SC, BCC and FCC\[13,15\]

\[
\begin{align*}
SC : l(r_0) &= -\frac{V b_2}{2N}, \quad r_0 \frac{\partial l}{\partial r} \bigg|_{r = r_0} = -\frac{V b_1}{N}, \\
BCC : l(r_0) &= -\frac{3V b_1}{8N}, \quad r_0 \frac{\partial l}{\partial r} \bigg|_{r = r_0} = \frac{3V}{8N} (b_1 - 3b_2), \\
FCC : l(r_0) &= \frac{V}{2N} \left( \frac{b_2}{2} - b_1 \right), \quad r_0 \frac{\partial l}{\partial r} \bigg|_{r = r_0} = \frac{V}{N} \left( b_1 - \frac{3b_2}{2} \right).
\end{align*}
\]

Here, we neglected the quadrupole contribution to the magnetoelastic energy\[13\]. This approximation is reasonable when \( q(r_0) \ll l(r_0) \). In Section \[3\] we show that BCC Fe and FCC Ni fulfill this condition. Next, as we did previously, inserting Eq. \[15\] into the Bethe-Slater curve and its derivative, and setting \( \delta_q = r_0 \) allow us to obtain

\[
\begin{align*}
\delta_q &= r_0, \\
\alpha_x &= e \left[ 2l(r_0) - r_0 \frac{\partial l}{\partial r} \bigg|_{r = r_0} \right], \\
\gamma_q &= \frac{r_0 \frac{\partial l}{\partial r} \bigg|_{r = r_0}}{r_0^2} - 2l(r_0).
\end{align*}
\]

These are the Bethe-Slater parameters in terms of \( b_1 \) and \( b_2 \) (via Eq. \[15\]) to model the magnetostriiction within the Néel model. Notice that a similar procedure to this one could be followed if a function with three parameters different to the Bethe-Slater curve is chosen to describe the dipole and quadrupole terms of Néel interaction in SD-MD simulations.

### III. SPIN-LATTICE MODEL FOR BCC Fe AND FCC Ni

In this section, we build a SD-MD model for BCC Fe and FCC Ni based on the methodology presented in Section \[2\].
The construction of the model is splitted into the following stages in order to compute each term in Eq[1]

A. Interatomic potential and exchange interaction

In the model we set the modified embedded atom method (MEAM) potentials developed by Asadi et al[25] and Lee et al[26] for the interatomic potential \( V(r_{ij}) \) of BCC Fe and FCC Ni, respectively. These potentials give an elastic tensor very close to the experimental one at zero-temperature. We also set the values obtained by Tranchida et al[29] for the parametrization of exchange interaction \( J(r_{ij}) \) through the Bethe-Slater curve (\( \alpha_j, \gamma_j \) and \( \delta_j \)). These values are shown in Table [1].

For the magnetic moment we set the experimental value \( \mu = 2.22 \mu_B \) and \( 0.606 \mu_B \) for Fe and Ni, respectively[22].

Let’s now find the equilibrium volume and bulk modulus given by the model including only the MEAM potential and exchange interaction. To do so, we compute the energy of a set of conventional unit cells with different volume using the software LAMMPS[30] with the SPIN package[31] and we fit it to the Murnaghan equation of state (EOS)[32,33,34]. We verify that the pressure in the selected equilibrium state is lower than \( 5 \times 10^{-5} \) GPa. Here, it is important to include the offset in the exchange interaction (see Eq[2]) in order to have zero-pressure at the minimum of the total energy[35]. In Fig[1] we present the calculation of the energy versus volume curve for the conventional unit cell (2 atoms/cell for BCC Fe and 4 atoms/cell for FCC Ni). The equilibrium volume and bulk modulus found with this procedure is \( V_0 = 11.586754 \) Å\(^3\)/atom and \( B = 166.73 \) GPa for BCC Fe, and \( V_0 = 10.903545 \) Å\(^3\)/atom and \( B = 188.85 \) GPa for FCC Ni. Hence, the equilibrium distance to the first nearest neighbor is \( r_0 = 2.4690386 \) Å for BCC Fe, and \( 2.4890153 \) Å for FCC Ni.

B. Néel energy

Now, we are in a position to calculate the Bethe-Slater parameters for the dipole and quadrupole terms of the Néel interaction given by Eqs.[15] and [16] respectively. Firstly, we notice that a key quantity in these equations is the equilibrium distance to the first nearest neighbors \( r_0 \), which obviously depends on the Néel interaction. Fortunately, the energy of the dipole and quadrupole terms of the Néel interaction for Fe and Ni are of the order of \( \mu eV/atom \) (see Fig[2]), so that they are much lower than the total energy (eV/atom). As a result, these terms only induce a very small change in \( r_0 \) when they are included in the SD-MD model. This fact allows us to use \( r_0 \) given by the SD-MD model including only the MEAM potential and exchange interaction to calculate the Bethe-Slater parameters for the dipole and quadrupole terms of the Néel interaction. Hence, according to Eqs.[15] and [16] we can set \( \delta_\lambda = \delta_\gamma = r_0 = 2.4690386 \) Å for BCC Fe, and \( \delta_\lambda = \delta_\gamma = 2.4890153 \) Å for FCC Ni.

Once \( r_0 \) is determined, we calculate \( \alpha_q \) and \( \gamma_q \) using Eqs.[9,10,11] and [13]. Here, we set the experimental values of \( K_1 \) and \( (1/K_1)(\partial K_1/\partial \mu) \) approximately at zero-temperature, that is,

\[
K_1 = 55 \text{ KJ/m}^3 \quad \text{and} \quad (1/K_1)(\partial K_1/\partial \mu) = -7.3 \times 10^{-2} \text{ GPa}^{-1}
\]

for BCC Fe, and \( K_1 = -126 \text{ KJ/m}^3 \) and \( (1/K_1)(\partial K_1/\partial \mu) = -2.8 \times 10^{-2} \text{ GPa}^{-1} \) for FCC Ni. As we see in Eq[13] we also need the bulk modulus. In principle we could set its experimental value or the one given by the EOS of this SD-MD model. In this work we choose the second option in order to describe more accurately the relation between volume and pressure of the SD-MD model. Inserting all these quantities in Eq[13] via Eqs.[9] and [10] leads to \( \alpha_q = 28.5189 \mu eV/\text{atom} \) and \( \gamma_q = 1.05331 \) for BCC Fe, and \( \alpha_q = -49.1335 \mu eV/\text{atom} \) and \( \gamma_q = 1.1186 \) for FCC Ni.

Lastly, we calculate the Bethe-Slater parameters for the dipole term \( (\alpha_i, \gamma_i) \) using Eqs.[15] and [16]. In this case we need the values of the anisotropic magnetoelastic constants \( \lambda_{b1} \) and \( \lambda_{b2} \). These constants are related to the magnetostrictive coefficients \( \lambda_{001} \) and \( \lambda_{111} \) and elastic constants \( c_{ij} \) via[34,35]

\[
b_1 = -\frac{3}{2} \lambda_{001} (c_{11} - c_{12}),
\]

\[
b_2 = -3 \lambda_{111} c_{44}.
\]

To calculate \( b_1 \) and \( b_2 \) we use the experimental magnetostrictive coefficients \( \lambda_{001} = 26 \times 10^{-6} \) and \( \lambda_{111} = -30 \times 10^{-6} \) for BCC Fe, and \( \lambda_{001} = -60 \times 10^{-6} \) and \( \lambda_{111} = -35 \times 10^{-6} \) for FCC Ni at zero-temperature[36]. For the values of the elastic constants we have two options: (i) the experimental ones at zero-temperature or (ii) the calculated ones with the SD-MD model including only the MEAM potential and ex-
change interaction at zero-temperature. Choosing the first option would give a SD-MD model with exactly the same magnetoelastic energy as in the experiment, while the second option would give a SD-MD model with magnetostrictive coefficients slightly closer to the experiment. To clarify this point, we evaluated the elastic tensor calculated with software AELAS interfaced with LAMMPS at the equilibrium volume \( v_0 \) including the MEAM potential and exchange interaction. The developed interface between AELAS and LAMMPS is available on GitHub repository. Here, we make use of the program Atomsk to convert some input files. As we see in Table I, the SD-MD model gives a very similar elastic tensor to the experiment. Therefore, both options lead to very similar results. In this work, we choose the second option since it gives a bit more accurate measurable macroscopic property like magnetostriction. Doing so, we get \( b_1 = -3.74166 \) MJ/m\(^3\) and \( b_2 = 10.4643 \) MJ/m\(^3\) for BCC Fe, and \( b_1 = 10.0611 \) MJ/m\(^3\) and \( b_2 = 13.9398 \) MJ/m\(^3\) for FCC Ni. If we insert these values in Eq.16 via Eq.15, then we obtain \( \alpha_l = 392.747 \mu eV/\)atom and \( \gamma_l = 0.824409 \) for BCC Fe, and \( \alpha_l = 179.396 \mu eV/\)atom and \( \gamma_l = 1.398484 \) for FCC Ni. The Bethe-Slater parameters for the constructed SD-MD models are shown in Table I. The evaluation of the quadrupole and dipole Bethe-Slater function at equilibrium shows that the Néel interaction Eq.3 in the SD-MD simulation is correct. To this end, we propose some tests by comparing the numerical results of the SD-MD simulation with simple analytical solutions. For instance, if we consider a BCC structure with Néel interactions up to first nearest neighbor in a collinear state along \( s = (0,0,1) \), then from Eq.5 we have

\[
\mathcal{H}_{\text{Néel}}(0,0,1) = \frac{16Nq(r_0)}{45},
\]

where \( N \) is the number of atoms in the system, \( r_0 \) is the distance to nearest neighbor that is related to the lattice parameter \( a \) via \( r_0 = a\sqrt{3}/2 \). This equation allows to verify the quadrupole term. In case we apply to this system a tetragonal deformation, then from Eq.5 we obtain

\[
\mathcal{H}_{\text{Néel}}(0,0,1) = -4NI(r_0) \left[ \frac{\left(\frac{c}{a}\right)^2}{2 + \left(\frac{c}{a}\right)^2} - \frac{1}{3} \right] - \frac{16Nq(r_0)}{35} \left[ \frac{2\left(\frac{c}{a}\right)^4 - 12\left(\frac{c}{a}\right)^2 + 3}{2 + \left(\frac{c}{a}\right)^2} \right],
\]

where

\[
r_0 = a \sqrt{\frac{2 + \left(\frac{c}{a}\right)^2}{2}}.
\]

This equation allows to check both the dipole and quadrupole terms. In the limit \( c/a \to 1 \), the Eq.19 becomes Eq.18 ensuring the continuity of the Néel energy under structure deformation. In Fig.2, we verify that the calculation of the Néel energy with LAMMPS is the same to Eqs.18 and 19 using the Bethe-Slater parameters of BCC Fe given in Table I. Similar tests could also be performed for other magnetic moment directions and deformations.

### Table I. Parameters of the SD-MD model for BCC Fe and FCC Ni.

| SD-MD model parameters | BCC Fe | FCC Ni |
|------------------------|--------|--------|
| \( \alpha_l \) (\( \mu eV/\)atom) | 25.498\(^a\) | 9.73\(^a\) |
| \( \gamma_l \) | 0.281\(^a\) | 0.00011\(^a\) |
| \( \delta_l \) (\( \AA \)) | 1.999\(^a\) | 1.233\(^a\) |
| \( R_{c,f} \) (\( \AA \)) | 4.5\(^a\) | 4.5\(^a\) |
| \( \alpha_q \) (\( \mu eV/\)atom) | 392.747 | 179.396 |
| \( \gamma_q \) | 0.824409 | 1.398484 |
| \( \delta_q \) (\( \AA \)) | 2.4690386 | 2.4890153 |
| \( R_{c,q} \) (\( \AA \)) | 2.6 | 2.6 |

\(^a\)Ref.25

### IV. RESULTS

#### A. Tests of the Néel interaction

Before evaluating the magnetoelastic properties of the SD-MD model, it is convenient to check that the implementation of the Néel interaction Eq.5 in the SD-MD simulation is correct. To this end, we propose some tests by comparing the numerical results of the SD-MD simulation with simple analytical solutions. For instance, if we consider a BCC structure with Néel interactions up to first nearest neighbor in a collinear state along \( s = (0,0,1) \), then from Eq.5 we have

\[
\mathcal{H}_{\text{Néel}}(0,0,1) = \frac{16Nq(r_0)}{45},
\]

where \( N \) is the number of atoms in the system, \( r_0 \) is the distance to nearest neighbor that is related to the lattice parameter \( a \) via \( r_0 = a\sqrt{3}/2 \). This equation allows to verify the quadrupole term. In case we apply to this system a tetragonal deformation, then from Eq.5 we obtain

\[
\mathcal{H}_{\text{Néel}}(0,0,1) = -4NI(r_0) \left[ \frac{\left(\frac{c}{a}\right)^2}{2 + \left(\frac{c}{a}\right)^2} - \frac{1}{3} \right] - \frac{16Nq(r_0)}{35} \left[ \frac{2\left(\frac{c}{a}\right)^4 - 12\left(\frac{c}{a}\right)^2 + 3}{2 + \left(\frac{c}{a}\right)^2} \right],
\]

where

\[
r_0 = a \sqrt{\frac{2 + \left(\frac{c}{a}\right)^2}{2}}.
\]

This equation allows to check both the dipole and quadrupole terms. In the limit \( c/a \to 1 \), the Eq.19 becomes Eq.18 ensuring the continuity of the Néel energy under structure deformation. In Fig.2, we verify that the calculation of the Néel energy with LAMMPS is the same to Eqs.18 and 19 using the Bethe-Slater parameters of BCC Fe given in Table I. Similar tests could also be performed for other magnetic moment directions and deformations.
TABLE II. Calculated and experimental elastic constants, magnetostrictive coefficients, MCA, and MCA under hydrostatic pressure for BCC Fe and FCC Ni at zero-temperature.

| Material | Elastic constants | MagnetostRICTIVE coefficients | MCA | MCA vs P |
|----------|-------------------|-------------------------------|-----|----------|
|          | SD-MD (GPa)       | Exp. (GPa)                    | SD-MD (x 10⁻⁶) | Exp. (x 10⁻⁶) | Expt. |
| BCC Fe   |                  |                              |     |          |
| c₁₁      | 230.0            | 230ₐ                         | λ₀₀₁ | 25.9     | 26°C   |
| c₁₂      | 134.1            | 135ₐ                         | λ₁₁₁ | -30.3    | -30°C  |
| c₄₄      | 116.3            | 117ₐ                         |      |          |

| FCC Ni   |                  |                              |     |          |
| c₁₁      | 263.9            | 261.2ₜ                         | λ₀₀₁ | -61.9    | -60°C  |
| c₁₂      | 152.1            | 150.ₜ                         | λ₁₁₁ | -35.4    | -35°C  |
| c₄₄      | 132.8            | 131.ₜ                         |      |          |

Ref [33], Ref [34], Ref [35], Ref [36], Ref [37], Ref [38].

B. Magnetic properties at zero-temperature

In this section, we evaluate the magnetization and MCA under pressure, and magnetostrictive coefficients at zero-temperature given by the developed SD-MD models for BCC Fe and FCC Ni in Section III. We include MEAM potentials, exchange and Néel energies in the following calculations. Only magnetic collinear states will be used since we are interested in properties at zero-temperature. All simulations are performed with the SPIN package of LAMMPS [39].

1. Ground state

Firstly, we determine the equilibrium volume of the full SD-MD model (including the Néel interaction) for the conventional unit cell of BCC Fe and FCC Ni. To this end, we calculate the energy versus volume curve, and we fit it to the Murnaghan EOS in the same way as it was done in Fig 1 previously. Here, we also set the magnetic moments along the easy direction ([1,0,0] for BCC Fe and [1,1,1] for FCC Ni) in order to get the minimum energy of the quadrupole term of Néel interaction. The equilibrium volume found with this procedure is \(v_0 = 11.5867635 \text{ Å}^3\) for BCC Fe, and \(v_0 = 10.9035445 \text{ Å}^3\) for FCC Ni. We verify that pressure is lower than \(5 \times 10^{-5}\) GPa in these equilibrium states. As we anticipated in Section III the dipole and quadrupole Néel interactions induce a very small change in the equilibrium volume when is included in the SD-MD model.

2. MagnetoCristalline anisotropy

Next, we compute the MCA energy at this equilibrium volume by setting the magnetic moment along different directions in the XY plane. In Fig 3 we show a comparison between the MCA energy calculated by SD-MD simulations with LAMMPS and Eq (7) using the experimental value \(K_1 = 55 \text{ KJ/m}^3\) for BCC Fe and \(K_1 = -126 \text{ KJ/m}^3\). The direct evaluation of \(K_1\) with the SD-MD model through Eq 8 gives 54.995 KJ/m³ for BCC Fe and -125.996 KJ/m³ for FCC Ni. As we see, the SD-MD model with the Bethe-Slater parameters given by Table I reproduces very well the first-order experimental MCA.

![FIG. 3](image)

FIG. 3. Calculation of the MCA energy for BCC Fe and FCC Ni with SD-MD simulation (blue points) and Eq (7) using the experimental \(K_1\) (red line). Magnetic moments are constrained on the XY plane.

Now we study the effects of hydrostatic pressure on the MCA for this SD-MD model. For easier comparison between the model and experiment, we first convert \((1/K_1) \partial K_1/\partial P\) to an integral form, that is,  
\[
\frac{1}{K_1} \frac{\partial K_1}{\partial P} = \zeta \quad \rightarrow \quad \int_{K_1(0)}^{K_1(P)} \frac{dK_1}{K_1} = \int_0^P \zeta dP,  \tag{21}
\]
where \(\zeta = -7.3 \times 10^{-2} \text{ GPa}^{-1}\) is the experimental value measured up to \(P = 0.5 \text{ GPa}\) at \(T=77K\) for BCC Fe [31], while for FCC Ni is \(\zeta = -2.8 \times 10^{-2} \text{ GPa}^{-1}\). Solving this integral we have  
\[
\frac{K_1(P)}{K_1(0)} = e^{\zeta P},  \tag{22}
\]

![FIG. 4](image)

FIG. 4. Calculation of \(K_1(P)/K_1(0)\) under hydrostatic pressure using the developed SD-MD model (blue dots) for BCC Fe and FCC Ni. The green and red lines stand for the experimental behaviour given by Eq 22 and its low-pressure approximation Eq 23, respectively [31].

```
where in the low pressure regime ($\zeta P \ll 1$) it can be written as

$$K_1(P)/K_1(0) \approx 1 + \zeta P + O(P^2).$$  \hspace{1cm} (23)

In Fig. 4, we show the ratio $K_1(P)/K(0)$ versus pressure generated by the SD-MD model of Fe and Ni, and the experimental behaviour given by Eq. 22 and its low-pressure approximation Eq. 23. The linear fitting to the data generated by the SD-MD model up to $P = 0.5$ GPa gives $(1/K_1)(\partial K_1/\partial P) = -7.27 \times 10^{-2}$ GPa$^{-1}$ for BCC Fe, and $-2.79 \times 10^{-2}$ GPa$^{-1}$ for FCC Ni, which is in very good agreement with the experimental values. Note that Eq. 22 and MCA results of the model beyond the range of pressure between 0GPa and 0.5GPa should be taken with caution due to the lack of experimental data.

![Graph](image)

FIG. 5. Calculation of $\beta$ cell length along SD-MD model up to $P$ behavior given by Eq. 22 and its low-pressure approximation Eq. 23. The linear fitting to the data generated by the SD-MD model beyond the range of pressure between 0GPa and 41GPa gives $K_1(P)/K(0) \approx 1 + \zeta P + O(P^2)$. Note that Eq. 22 and MCA results of the model beyond the range of pressure between 0GPa and 0.5GPa should be taken with caution due to the lack of experimental data.

3. Magnetostriction

Now, we compute the anisotropic magnetostrictive coefficients using the SD-MD model. To this end, we apply the method proposed by Wu and Freeman, as implemented in the program MAELAS. Namely, the anisotropic magnetostrictive coefficients for cubic systems (point groups 432, 43m, m3m) are calculated as

$$\lambda_{001} = \frac{4(l_{100}^0 - l_{101}^0)}{3(l_{100}^0 + l_{101}^0),} \lambda_{111} = \frac{4(l_{111}^0 - l_{111}^1)}{3(l_{111}^0 + l_{111}^1).} \hspace{1cm} (24)$$

where $l_{100}^0$ and $l_{101}^0$ are the equilibrium cell lengths along the length measuring direction $\vec{b} = (0, 0, 1)$ under a tetragonal deformation with collinear magnetic moment directions $\vec{s}_1 = (0, 0, 1)$ and $\vec{s}_2 = (1, 0, 0)$, respectively. Similarly, $l_{111}^0$ and $l_{111}^1$ are the equilibrium cell lengths along the length measuring direction $\vec{b} = (1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3})$ under a trigonal deformation with magnetic moment direction $\vec{s}_1 = (1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3})$ and $\vec{s}_2 = (1, 0, 0) \approx (1/\sqrt{2}, 0, -1/\sqrt{2})$, respectively. In order to obtain the equilibrium cell lengths $l_{100}^0$ and $l_{101}^0$, one needs to evaluate the energy for a set of volume-conserving tetragonal distorted unit cells. Next, the energy versus the cell length along $\vec{b} = (0, 0, 1)$ for each magnetic moment direction $\vec{s}_1 = (0, 0, 1)$ and $\vec{s}_2 = (1, 0, 0)$ is fitted to a

FIG. 6. Calculation of $\lambda_{111}$ for BCC Fe using MAELAS interfaced with LAMMPS. (top) Quadratic curve fit to the energy versus cell length along $\vec{b} = (1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3})$ with spin direction $\vec{s}_1 = (1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3})$ under a volume-conserving trigonal deformation. (bottom) Energy difference between states with spin directions $\vec{s}_2 = (1, 0, 0)$ and $\vec{s}_1 = (1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3})$ against the cell length along $\vec{b} = (1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3})$. The quadratic curve fit to the energy versus cell length along $\vec{b} = (0, 0, 1)$ with spin direction $\vec{s}_1 = (0, 0, 1)$ under a volume-conserving tetragonal deformation.

Now, we compute the anisotropic magnetostrictive coefficients using the SD-MD model. To this end, we apply the method proposed by Wu and Freeman, as implemented in the program MAELAS. Namely, the anisotropic magnetostrictive coefficients for cubic systems (point groups 432, 43m, m3m) are calculated as

$$\lambda_{001} = \frac{4(l_{100}^0 - l_{101}^0)}{3(l_{100}^0 + l_{101}^0),} \lambda_{111} = \frac{4(l_{111}^0 - l_{111}^1)}{3(l_{111}^0 + l_{111}^1).} \hspace{1cm} (24)$$

where $l_{100}^0$ and $l_{101}^0$ are the equilibrium cell lengths along the length measuring direction $\vec{b} = (0, 0, 1)$ under a tetragonal deformation with collinear magnetic moment directions $\vec{s}_1 = (0, 0, 1)$ and $\vec{s}_2 = (1, 0, 0)$, respectively. Similarly, $l_{111}^0$ and $l_{111}^1$ are the equilibrium cell lengths along the length measuring direction $\vec{b} = (1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3})$ under a trigonal deformation with magnetic moment direction $\vec{s}_1 = (1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3})$ and $\vec{s}_2 = (1, 0, 0) \approx (1/\sqrt{2}, 0, -1/\sqrt{2})$, respectively. In order to obtain the equilibrium cell lengths $l_{100}^0$ and $l_{101}^0$, one needs to evaluate the energy for a set of volume-conserving tetragonal distorted unit cells. Next, the energy versus the cell length along $\vec{b} = (0, 0, 1)$ for each magnetic moment direction $\vec{s}_1 = (0, 0, 1)$ and $\vec{s}_2 = (1, 0, 0)$ is fitted to a
where $\tilde{a}_j$, $\tilde{b}_j$ and $\tilde{c}_j$ are fitting parameters. The minimum of this quadratic function for magnetic moment direction $\mathbf{s}_1(2)$ corresponds to $E(001) = -\tilde{b}_1(2)/(2\tilde{a}_1(2))$, and it is the equilibrium cell length. Similarly, the equilibrium cell lengths $l_{111}^1$ and $l_{111}^2$ are obtained by applying a set of volume-conserving trigonal deformations, and performing a quadratic fitting of the energy versus the cell length along $\mathbf{\beta} = (1/\sqrt{3},1/\sqrt{3},1/\sqrt{3})$ with magnetic moment directions $\mathbf{s}_1 = (1/\sqrt{3},1/\sqrt{3},1/\sqrt{3})$ and $\mathbf{s}_2 = (1/\sqrt{3},0,-1/\sqrt{3})$.

FIG. 7. Calculation of $\lambda_{001}$ for FCC Ni using MAELAS interfaced with LAMMPS. (top) Quadratic curve fit to the energy versus cell length along $\mathbf{\beta} = (0,0,1)$ with spin direction $\mathbf{s}_1 = (0,0,1)$ under a volume-conserving tetragonal deformation. (bottom) Energy difference between states with spin directions $\mathbf{s}_2 = (1,0,0)$ and $\mathbf{s}_1 = (0,0,1)$ against the cell length along $\mathbf{\beta} = (0,0,1)$.

We have developed an interface between the software MAELAS and LAMMPS in order to apply this method and extract the magnetostrictive coefficients. This interface is publicly available on GitHub repository. In Fig. 5 we show the quadratic curve fit to the energy versus cell length along [0,0,1] with magnetic moment direction $\mathbf{s}_1 = (0,0,1)$ to calculate $\lambda_{001}$ for BCC Fe. We also plot the energy difference between states with spin directions $\mathbf{s}_1 = (1,0,0)$ and $\mathbf{s}_2 = (0,0,1)$ against the cell length along [0,0,1]. The corresponding plot for $\lambda_{111}$ is presented in Fig. 6. We obtain $\lambda_{001} = 25.9 \times 10^{-6}$ and $\lambda_{111} = -30.3 \times 10^{-6}$, while the experimental values at $T = 4.2$K are $\lambda_{001} = 26 \times 10^{-6}$ and $\lambda_{111} = -30 \times 10^{-6}$. The results for FCC Ni are plotted in Figs. 7 and 8. Here, we get $\lambda_{001} = -61.9 \times 10^{-6}$ and $\lambda_{111} = -35.4 \times 10^{-6}$, while the experimental values at $T = 4.2$K are $\lambda_{001} = -60 \times 10^{-6}$ and $\lambda_{111} = -35 \times 10^{-6}$. Therefore, the developed SD-MD model for Fe and Ni also exhibits magnetostrictive properties very similar to the experiment. Additionally, this calculation reveals that the method proposed by Wu and Freeman is an excellent approach to obtain the magnetostrictive coefficients as soon as both the elastic and magnetoelastic energies are properly described by the model. This fact could not be verified before for $\lambda_{111}$ of BCC Fe due to the lack of accuracy of first-principle calculation. In Table I we present a summary of the results given by the SD-MD model for the MCA, MCA under hydrostatic pressure, and magnetostrictive coefficients.

FIG. 8. Calculation of $\lambda_{111}$ for FCC Ni using MAELAS interfaced with LAMMPS. (top) Quadratic curve fit to the energy versus cell length along $\mathbf{\beta} = (1/\sqrt{3},1/\sqrt{3},1/\sqrt{3})$ with spin direction $\mathbf{s}_1 = (1/\sqrt{3},1/\sqrt{3},1/\sqrt{3})$ under a volume-conserving trigonal deformation. (bottom) Energy difference between states with spin directions $\mathbf{s}_2 = (1/\sqrt{3},0,-1/\sqrt{3})$ and $\mathbf{s}_1 = (1/\sqrt{3},1/\sqrt{3},1/\sqrt{3})$ against the cell length along $\mathbf{\beta} = (1/\sqrt{3},1/\sqrt{3},1/\sqrt{3})$.

V. CONCLUSIONS

Many aspects of magnetoelastic phenomena are not fully understood yet due to the complexity of the materials at large
scale. Advanced modeling techniques and associated numerical tools based on a bottom-up multiscale approach could help to get a better understanding of magnetoelastic phenomena in magnetic materials across length scales. In this sense the SD-MD simulations using the Néel model could play an important role linking the atomic and macroscopic scales. Aiming at exploring this possibility, we showed a general methodology to build SD-MD models to describe MCA under hydrostatic pressure and anisotropic magnetostriction. To illustrate the method, we successfully applied it to BCC Fe and FCC Ni at zero-temperature.

We aim at transposing our methodology to other materials and crystal structures. For example, in magnetic oxides and 4-f magnets, the spin-orbit coupling can correspond to energies orders of magnitude larger than in magnetic 3-d metals. Our approach could be used to map the subsequent interactions and build meso-scale models that will help reveal the influence of magnetism on large-scale thermo-elastic materials properties.

Although this work focused on bulk magnetoelasticity, similar effects have been shown to be important for smaller scale, fine-size systems. Previous studies have been investigating the relevance of the Néel model to simulate surface effects in 3-d magnetic metals. Future work could leverage our framework to develop surface interaction models for spin-lattice simulations of magnetic nanoparticles.

These results raise interesting questions for future research on how these models will perform at finite temperature, and under magnetic field and stress.

**ACKNOWLEDGEMENT**

Authors acknowledge the European Regional Development Fund in the IT4Innovations national supercomputing center - path to exascale project, project number CZ.02.1.01/0.0/0.0/16-013/0001791 within the Operational Programme Research, Development and Education. DL acknowledges the Czech Science Foundations grant No. 17-23964S. This work was also supported by the Donau project No. 8X20050. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA-0003525. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

**APPENDIX**

**Appendix A: Derivation of $\partial q/\partial r$**

In this appendix we show the steps to obtain the final expression for $\partial q/\partial r$ given by Eq. (10). Firstly, we write the derivative of $q(r)$ with respect to the first nearest neighbor distance $r$ in Eq. (9) as

$$q(r) = -\frac{\xi V K_1}{N} \rightarrow r_0 \frac{\partial q}{\partial r} \bigg|_{r=r_0} = -\frac{\xi r_0}{N} \frac{\partial (V K_1)}{\partial r} \bigg|_{r=r_0}, \quad (A1)$$

where $r_0$ is the equilibrium distance to the first nearest neighbors, $N$ is the number of atoms in the volume $V$, and $\xi$ is equal to $-1/2$, 9/16, and 1 for SC, BCC and FCC, respectively. Next, we work out this equation in the following way

$$r_0 \frac{\partial q}{\partial r} \bigg|_{r=r_0} = -\frac{\xi r_0}{N} \frac{\partial (V K_1)}{\partial r} \bigg|_{r=r_0} = -\frac{\xi r_0}{N} \left[ K_1 + \frac{V \partial K_1}{\partial r} \right]_{r=r_0}$$

$$= -\frac{\xi r_0}{N} \frac{\partial V}{\partial r} \left[ K_1 + \frac{V \partial K_1}{\partial r} \right]_{r=r_0}$$

$$= -\frac{\xi r_0}{N} \frac{\partial V}{\partial r} \left[ K_1 + \frac{V \partial P}{\partial r} \frac{\partial K_1}{\partial P} \right]_{r=r_0}, \quad (A2)$$

where

$$SC: \quad \frac{\xi r_0}{N} \frac{\partial V}{\partial r} \bigg|_{r=r_0} = -\frac{3}{2} \sqrt{2}$$

$$BCC: \quad \frac{\xi r_0}{N} \frac{\partial V}{\partial r} \bigg|_{r=r_0} = \frac{3\sqrt{3}}{4} \sqrt{2}$$

$$FCC: \quad \frac{\xi r_0}{N} \frac{\partial V}{\partial r} \bigg|_{r=r_0} = \frac{3}{\sqrt{2}}$$

Lastly, we make use of the definition of the bulk modulus $B = -V(\partial^2 V/\partial P^2)$ in Eq. (A2) so, we obtain Eq. (10)
50 N. J. Jones, G. Petculescu, M. Wun-Fogle, J. B. Restorff, A. E. Clark, K. B. Hathaway, D. Schlagel, and T. A. Lograsso, Journal of Applied Physics 117, 17A913 (2015), https://doi.org/10.1063/1.4916541, URL https://doi.org/10.1063/1.4916541.

51 T. Burkert, O. Eriksson, P. James, S. I. Simak, B. Johansson, and L. Nordström, Phys. Rev. B 69, 104426 (2004), URL https://link.aps.org/doi/10.1103/PhysRevB.69.104426.

52 R. Yanes, O. Chubykalo-Fesenko, H. Kachkachi, D. Garanin, R. Evans, and R. Chantrell, Physical review B 76, 064416 (2007).

53 R. Skomski, IEEE transactions on magnetics 34, 1207 (1998).

54 G. Dos Santos, R. Aparicio, D. Linares, E. Miranda, J. Tranchida, G. Pastor, and E. Bringa, Physical Review B 102, 184426 (2020).