Strain control of the Néel vector in Mn-based antiferromagnets

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Control of the Néel vector in antiferromagnetic materials is one of the challenges preventing their use as active device components. Several methods have been investigated such as exchange bias, electric current, and spin injection, but little is known about strain-mediated anisotropy. This study of the antiferromagnetic $L1_{0}$-type MnX alloys MnIr, MnRh, MnNi, MnPd, and MnPt shows that a small amount of strain effectively rotates the direction of the Néel vector by 90° for all of the materials. For MnIr, MnRh, MnNi, and MnPd, the Néel vector rotates within the basal plane. For MnPt, the Néel vector rotates from out-of-plane to in-plane under tensile strain. The effectiveness of strain control is quantified by a metric of efficiency and by direct calculation of the magnetostriction coefficients. The values of the magnetostriction coefficients are comparable with those from ferromagnetic materials. These results indicate that strain is a mechanism that can be exploited for control of the Néel vectors in this family of antiferromagnets.

There has been a rapidly increasing interest in the use of antiferromagnetic (AFM) materials for use as active device elements\textsuperscript{1–3}. AFMs are insensitive to parasitic electromagnetic and magnetic interference. The dipolar coupling is minimal, since there is no net magnetic moment. Their lack of macroscopic magnetic fields allows AFM devices and interconnects to be highly scaled with reduced cross talk and insensitivity to geometrical anisotropy effects. AFM resonant frequencies and magnon velocities are several orders of magnitude higher than those in ferromagnetic materials, and these velocities correlate with similarly higher switching speeds\textsuperscript{3–5}. AFM metals and insulators are plentiful, and many have Néel temperatures well above room temperature, a requirement for compatibility with on-chip temperatures in current Si integrated circuits.

The high Néel temperatures of the Mn-based equiatomic alloys such as MnIr, MnRh, MnNi, MnPd, and MnPt make them suitable candidates for on-chip applications\textsuperscript{4}. Extensive research has been conducted on the electronic\textsuperscript{6–10}, magnetic\textsuperscript{6,9–11}, and elastic properties\textsuperscript{12,13} of these materials. The spins on the Mn atoms are antiferromagnetically coupled with each other in the basal plane, and each plane is coupled ferromagnetically as shown in Fig. 1.

The positive attributes of speed, scaling, and robustness to stray fields are accompanied by the challenges of manipulating and detecting the antiferromagnetic states. There are several methods to control the magnetic properties of AFM materials such as with exchange bias\textsuperscript{4}, the use of electric current\textsuperscript{14}, and strain induced by a piezoelectric material\textsuperscript{15,16}. The recent experimental demonstration of strain control of the Néel vector in MnPt\textsuperscript{16}, provides timely motivation for a theoretical study of strain-mediated magnetic anisotropy in the MnX AFM materials. Density functional theory (DFT) is used to analyze the effect of strain on the magnetic anisotropy. The effectiveness of strain control is quantified by a metric of efficiency and by calculation of the magnetostriction coefficients.

First principles calculations are performed as implemented in the Vienna Ab initio Simulation Package (VASP)\textsuperscript{17} to investigate the effect of strain on the magnetic anisotropy of $L1_{0}$-ordered bulk MnIr, MnRh, MnNi, MnPd, and MnPt. Projector augmented-wave (PAW) potentials\textsuperscript{18} and the generalized gradient approximation (GGA) parameterized by Perdew-Burke-Ernzerhof (PEB) were employed\textsuperscript{19}. Depending on the materials, different cut-off energies (typically ranging from 420 eV to 450 eV) and k-points grids were used in order to ensure the total energy converged within $10^{-7}$ eV per unit cell. The initial equilibrium structure consists of a tetrag-
TABLE I: Calculated structure and local magnetic moment of the \(L1_0\)-type MnX alloys in the absence of strain.

|       | \(a (\text{Å})\) | \(b (\text{Å})\) | \(c (\text{Å})\) | \(\mu_{\text{Mn}} (\mu_B)\) |
|-------|------------------|------------------|------------------|--------------------------|
| MnIr  | 3.84             | 3.84             | 3.64             | 2.8                      |
| MnRh  | 3.85             | 3.85             | 3.62             | 3.1                      |
| MnNi  | 3.62             | 3.62             | 3.58             | 3.2                      |
| MnPd  | 3.99             | 3.99             | 3.69             | 3.8                      |
| MnPt  | 3.98             | 3.98             | 3.71             | 3.7                      |

The strain is defined as, strain = \((a - a_0)/a_0 \times 100\%\), where \(a\) and \(a_0\) are the lattice constants with and without strain, respectively. With the relaxed structure, the spin-polarized self-consistent calculation is performed to obtain the charge density. Finally, the magnetic anisotropy energies are determined by calculating the total energies for different Néel vector directions including spin orbit coupling. Table I shows the lattice constants and the magnetic moments of the Mn site in MnX without strain. All of the values are very close to those from previous results\(^\text{12,13}\). The local magnetic moments of the X site are zero for all materials.

Figures 2–6 show the differences in the total energies as a function of the strain for MnIr, MnRh, MnNi, MnPd, and MnPt, respectively, where \(E_{abc}\) is the ground state energy with the Néel vector along the \([abc]\) direction. The reference energy levels from each figure, which are indicated by the solid black lines, are \(E_{001}\) for MnPt and \(E_{110}\) for the other materials. The reference energies are the lowest energy state, which means MnIr, MnRh, MnNi, and MnPd have in-plane anisotropy and MnPt has out-of-plane anisotropy without strain. This is consistent with experimental results\(^\text{11}\). To show the energy differences more clearly as the strain changes, the reference level is taken at each value of the applied strain. At zero strain, there is no energy difference between \(E_{100}\) and \(E_{010}\) because of the symmetry of all of the materials.

Figures 2–5 show that sweeping the strain from negative (compressive) to positive (tensile) causes a 90° rotation of the Néel vector in the \(ab\)-plane for the four materials MnIr, MnRh, MnNi, and MnPd. However, the alignment of the Néel vector with compressive or tensile strain depends on the specific material. MnIr and MnRh behave like magnets with a positive magnetostriction coefficient, since tensile strain along \([100]\) causes the Néel vector to align in the \([100]\) direction. On the other hand, MnNi and MnPd behave like magnets with a negative magnetostriction coefficient, since tensile strain along \([100]\) causes the Néel vector to align in the \([010]\) direction\(^\text{20}\).
FIG. 5: MnPd energy differences $E_{abc} - E_{110}$ for the 3 different orientations of the Néel vector as indicated by the labels.

FIG. 6: MnPt energy differences $E_{abc} - E_{110}$ for the 3 different orientations of the Néel vector as indicated by the labels.

MnPt is unique among the 5 materials. In equilibrium, in the absence of strain, the Néel vector has perpendicular anisotropy. Under compressive (negative) strain along the [100] axis, the Néel vector remains out-of-plane. Under tensile strain along [100], the Néel vector switches from out-of-plane [001] to in-plane aligning in the [010] direction.

For applications, it is useful to quantify the efficiency with which strain rotates the Néel vector and to determine the magnetostriction coefficient from the ab initio calculations. The internal efficiency is defined as

$$\text{Efficiency}(\%) = \left( \frac{E_{abc} - E_{a'b'c'}}{E_{\text{total}} - E_{\text{total}(0)}}\right) \times 100, \quad (1)$$

where the total energies $E_{abc}$ and $E_{a'b'c'}$ are defined in the same way as above, i.e. the total energies in the presence of strain with the Néel vector oriented along $[abc]$ or $[a'b'c']$, respectively. The denominator in the Eq. (1) is the total energy change induced by the strain. For MnIr, MnRh, MnNi, and MnPd, $E_{abc}$ and $E_{a'b'c'}$ are $E_{010}$ and $E_{001}$, respectively. For MnPt, $E_{abc}$ and $E_{a'b'c'}$ are $E_{010}$ and $E_{001}$, respectively. The numerator and denominator of Eq. (1) are plotted as a function of strain in Figs. 7-11(a), and the resulting efficiencies are plotted as a function of strain in Figs. 7-11(b). The changes in the total energies, shown as red curves in Figs. 7-11(a), are parabolic so that they can be considered as the strain energy proportional to the square of the applied strain. On the other hand, the differences between two energies (the black curves in Figs. 7-11(a)) are approximately linear under small strain (<1%). Therefore, the efficiency decreases sharply as the amount of strain

FIG. 7: MnIr strain energies and efficiency versus strain. (a) The energy difference between two different Néel vector orientations (black) as shown by the left axis, and the change in total energy (red) as shown by the right axis. (b) The efficiency as a function of the strain.

FIG. 8: MnRh strain energies and efficiency versus strain. (a) The energy difference between two different Néel vector orientations (black) as shown by the left axis, and the change in total energy (red) as shown by the right axis. (b) The efficiency as a function of the strain.

FIG. 9: MnNi strain energies and efficiency versus strain. (a) The energy difference between two different Néel vector orientations (black) as shown by the left axis, and the change in total energy (red) as shown by the right axis. (b) The efficiency as a function of the strain.
increases. At 0% change in total energy (red) as shown by the right axis. (b) The efficiency as a function of the strain.

FIG. 11: MnPt strain energies and efficiency versus strain. (a) The energy difference between two different Neel vector orientations (black) as shown by the left axis, and the change in total energy (red) as shown by the right axis. (b) The efficiency as a function of the strain.

In summary, the Neel vectors of MnIr, MnRh, MnNi, and MnPd can be rotated 90° in the basal plane by applying in-plane strain. MnIr and MnRh behave like magnets with positive magnetostriction coefficients, since their Neel vectors align with tensile strain. MnNi and MnRh behave like magnets with negative magnetostriction coefficients, since their Neel vectors align with compressive strain. The internal efficiency of this process is highest for MnIr and it is equal to 20% at 0.5% strain. MnPt is unique among the 5 alloys in that its Neel vector aligns out-of-plane along the [001] axis in equilibrium. Applying a tensile strain along [100] rotates the Neel vector from out-of-plane [001] to in-plane [010]. The efficiency of this process at 0.5% tensile strain is 6%. Under compressive strain along [100], the Neel vector of MnPt remains out-of-plane [001]. The magnitudes of the calculated magnetostriction coefficients are comparable with those of ferromagnets, and they follow the same trends as the calculated efficiencies. For in-plane rotation of the Neel vector, MnIr has the highest magnetostriction coefficient of 241 ppm. The magnetostriction coefficient for out-of-plane rotation in MnPt is -196 ppm. These results suggest that strain can be an effective mechanism to control the Neel vectors in this family of antiferromagnets.

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Supplementary Information

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Figure S1 shows the change in the lattice constants in MnX alloys as a function of applied strain along the $a$ axis. The $a$ lattice parameter is linearly increased and the $b$ and $c$ lattice constants are relaxed. In figure S2, we show the calculated values of $K_{me}$ evaluated at all values of strain and make a linear fit to extract the slope, which is used as the term $\frac{K_{me}}{\varepsilon_{bb} - \varepsilon_{aa}}$ in the Eq. (2) in the main text. As mentioned in the main paper, the Young’s moduli were taken from previous results.$^{1,2}$ However, we were unable to find any values for the Young’s modulus of MnIr. To calculate the magnetostriction coefficient for MnIr, we adopted the bulk modulus from Materials Project$^3$ and used the relation $Y(GPa) = 3K(1-2\nu)$ where $Y$, $K$, and $\nu$ are the Young’s modulus, bulk modulus, and Poisson’s ratio, respectively.
FIG. S1: The lattice constants versus applied strain in (a) MnIr, (b) MnRh, (c) MnNi, (d) MnPd, and (e) MnPt.
FIG. S2: The magnetoelastic anisotropy constants versus applied strain in (a) MnIr, (b) MnRh, (c) MnNi, (d) MnPd, and (e) MnPt.
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