Evidence of ferromagnetic ground state and strong spin phonon coupling in Zr$_2$TiAl with bi-axial strain: first principles study

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Keywords: electronic structure, magnetism, Heusler alloy

Abstract

A detailed study on the inter-metallic alloy, Zr$_2$TiAl, has been carried out using first principles electronic structure calculations. We found that a small value of bi-axial strain/stress cause a phase change from anti-ferromagnetic (AFM) to ferromagnetic (FM) with a structural transition from face center cubic (fcc) to body center tetragonal (bct). Calculated electronic band structures show that all strained structures are metallic in nature with Zr-$d$ and Ti-$d$ orbital dominated energy bands near the Fermi level ($E_F$). The stability of FM phase is confirmed with phonon dispersion calculations by using density functional perturbation theory (DFPT). It has been observed that AFM state with both positive and negative bi-axial stress exhibits unstable modes while corresponding FM state shows no such instability. This clearly indicates the existence of large spin phonon coupling in this material.

1. Introduction

Alloys with combinations of Zr-Al and Ti-Al are having special interest to researchers because of their light weight, stiffness and oxidation resistance properties which are important properties to use a material in aerospace industry [1–7]. Compounds like Zr$_3$Al and Ti$_3$Al are having importance in high temperature applications [8–12]. Recently, Zirconium rich titanium aluminide, Zr$_2$TiAl has prepared by Sournadurai et al using arc-melting and vacuum annealing techniques [13]. Later, theoretical studies on the same compound confirmed an anti-ferromagnetic ground state with magnetic moment arising from Ti atom [14] and also observed a magnetic to non-magnetic phase transition under uniform compression.

It is well known that the external stimuli like, pressure, temperature, chemical doping etc lead to improve certain properties of parent materials. Sometimes it may lead to semi-metal to metal, magnetic to non-magnetic, normal to superconducting state transitions. Among those, bi-axial strain is one of the stimuli used to improve the material properties. This method is effectively used in tuning the ferroelectric and multiferroic properties of hetero-structures and thin-films [15–17]. In the case of BaTiO$_3$, bi-axial compressive strain helped to enhance ferroelectric properties [18]. In SrTiO$_3$, room temperature ferromagnetic ordering is observed with tensile strain [19].

Spin phonon coupling is commonly observed in transitional metal oxides such as in magnetoelectric multiferroic materials [20, 21]. Usually, in such materials, the interplay between the electric and magnetic order is described through the spin-phonon coupling.

In the present work, we show that as the bi-axial stress is applied, certain acoustic phonon mode become unstable for the (anti-ferromagnetic) AFM case, while no such instability is observed for the ferromagnetic (FM) case. This implies the AFM phase can be seen only at ambient condition.

In this work, we applied both bi-axial stress and strain to stabilize the system in ferromagnetic ground state and discussed the magnetic, electronic structure and vibrational properties in all applied strains/stress. The paper is organized as follows: section 2 presents computational details of the first-principles calculations. The
Zr$_2$TiAl was synthesized by Sournadurai et al. [3]. Ground state properties at ambient condition were reported in section 3. Results and discussions of ground state, electronic structure and vibrational properties are presented in section 3. Computational details

All the ground state and electronic structure calculations are performed by using Vienna ab-initio simulation package (VASP) [22, 23]. Firstly, structural optimizations were performed using the Perdew–Burke–Ernzerhof (PBE) functional [24], which is specifically customized for solids, that has been shown to yield structural data in agreement with experiment. The projector augmented wave (PAW) pseudopotential [25, 26] was used with an energy cutoff of 400 eV. The Brillouin zone has been sampled using a $12 \times 12 \times 12$ $\Gamma$-centered grid. Forces and total energies are converged to 0.01 eV/Å and $10^{-8}$ eV, respectively.

To investigate the dynamical stability of ambient and strained/stress structures, we have performed the phonon dispersion calculations by using force constants (VASP-DFPT) implemented in the Phonopy code [27]. A $2 \times 2 \times 2$ supercell created with 32 number of atoms to take into account of the long range inter atomic interactions to calculate the inter atomic forces by using VASP, with an energy cutoff 450 eV for planewave basis and an energy convergence criteria of $10^{-8}$ eV.

3. Results and discussion

3.1. Ground state properties at ambient

Zr$_2$TiAl was synthesized by Sournadurai et al. [13] in L2$_1$ phase with space group $Fm\overline{3}m$ (No: 225). Conventional and primitive crystal structures are given in figure 1. Atomic positions for 225 space group are Zr:8c (0.25, 0.25, 0.25), Ti:4b (0.5, 0.5, 0.5) and Al:4a (0.0, 0.0, 0.0). Later a theoretical study [14] on the same material confirmed anti-ferromagnetic (AFM) (figure 1(c)) ground state with energy difference 2.22 mRy/f.u. between AFM and FM configuration. The magnetic nature is arising from Ti atom. In the present work, we have started with the reproduction of ground state properties at ambient condition. Optimized lattice parameter details are tabulated in table 1 along with experimental and other theoretical data. Our calculated values are in good agreement with available data. Further, we have reproduced the AFM ground state and FM state with a energy difference $\approx 2.225$ mRy/f.u., which is in good agreement with earlier report [14]. This indicate our calculations are in correct direction.

3.2. Stabilizing the system in FM phase

A small disturbance in the system may lead to change in the ground state of the system as the energy difference between the AFM and FM is very small. In the application point of view, ferromagnetic materials have high priority in compare to AFM materials. The elements in the present alloy are low cost elements. So, it is worth enough, if we could get ferromagnetic ground state in the present material. We keep this as motivation and proceed further to achieve ferromagnetic ground state.

Here we have applied bi-axial strain/stress along $xy$-plane and allowed a change along $z$-axis. Experimentally, if we allow compression in two-dimensional on any system, suppose here $xy$, the other dimension will elongate accordingly. In the present case, we have fixed $a$ and $b$ lattice parameter values and allowed a change in the $c$ parameter accordingly in the relaxation process. A custom $z$-relaxation-only compilation of VASP was used to relax the lattice parameter $c$ along with all internal atomic coordinates. The value of bi-axial strain/stress is defined as $\varepsilon = (a-a_0)/a_0 \times 100\%$ where $a$ and $a_0$ are the in-plane lattice constants of the strained/stress and unstrained structures respectively. The relaxed parameters are given in table 2 for 1%, 2%, 3%, −1%, −2% and −3% stress values. For positive stress (1%, 2% and 3%), the lattice parameter $c$ is found to elongate and for negative stress (−1%, −2% and −3%) it is found to compressed. It is also observed that $c/a$ value is $>1$ for positive stress and $<1$ for negative stress values. After relaxation of the system with different strains/stress, it is observed that the space group of the system is found to change from 225 ($Fm\overline{3}m$) to 139 ($I4/\overline{mmm}$), from fcc to bct structure. The optimized atomic positions for the bct structure are Zr:4d (0.5, 0.0, 0.25), Ti:2b (0.5, 0.5, 0.0) and Al:2a (0.0, 0.0, 0.0). From the table 2, it is confirmed that the FM state is found to be stable in all the strain/stress cases and a large contribution of magnetic moment is arrived mainly from Ti atom and a small contribution from Zr atom. It is also observed that the magnetic moment of Ti is found to decrease with both positive and negative stress values. Total energy values with different stress values are plotted in figure 2(a) for both AFM and FM phases and confirmed that the FM phase is found to be stable in all stress cases. From the inset of the same plot, which is given only for FM case, same behavior observed with both positive and negative stress cases. Here the energy drop is mainly dependent on the structure of the system which is changing with the application of small stress. Other physical properties are not effected much with small stress except the magnetic phase. Electronic structure properties like band structure, density of states are already

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J. Phys. Commun. 3 (2019) 055010

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Figure 1. Crystal structure of Zr₂TiAl, (a) conventional, (b) primitive and (c) supercell case with indication of Ti planes along 111 direction.

Table 1. Calculated lattice parameters and magnetic moment of Zr₂TiAl at ambient pressure combined with experimental and other theory reports.

| Parameters                  | PAW-PBE | LDA⁶ | LDA-mag⁶ | GGA⁷  | GGA-mag⁷ | Experimental¹  |
|-----------------------------|---------|------|----------|--------|----------|----------------|
| Lattice parameter $a$ (Å)   | 6.837   | 6.668| 6.712    | 6.813  | 6.841    | 6.840          |
| Magnetic moment of Ti $\tau$ (μB) | 1.438   | —   | 0.8      | —      | 1.22     | —              |

Notes.
⁶ [13].
⁷ [14].

Table 2. Relaxed lattice parameters and magnetic moment of Zr₂TiAl in bi-axial stress. Calculated magnetic moments for Ti are given in the brackets.

| Bi-axial stress | $a = b$ (Å) | $c$ (Å) | $c/a$ | Volume Å³ | Energies (eV) AFM | FM |
|-----------------|-------------|--------|-------|-----------|-------------------|----|
| 1%              | 6.769       | 6.956  | 1.023 | 318.682   | −232.398 455 (1.189 μB) | −232.830 127 28 (1.421 μB) |
| 2%              | 6.700       | 7.077  | 1.056 | 317.729   | −232.364 353 82 (1.134 μB) | −232.776 908 67 (1.374 μB) |
| 3%              | 6.632       | 7.223  | 1.089 | 317.694   | −232.352 259 72 (1.046 μB) | −232.718 929 82 (1.277 μB) |
| −1%             | 6.905       | 6.731  | 0.975 | 320.976   | −232.405 248 21 (1.2 μB) | −232.827 367 87 (1.441 μB) |
| −2%             | 6.974       | 6.637  | 0.952 | 322.790   | −232.339 168 31 (1.181 μB) | −232.748 490 71 (1.435 μB) |
| −3%             | 7.042       | 6.544  | 0.929 | 324.536   | −232.217 409 82 (1.146 μB) | −232.604 118 36 (1.417 μB) |
reported [14] for ambient case. In the present work we have completely reproduced the ambient results but not reported here. It is worth enough to know the same details with applied strain/stress which causes AFM to FM phase transition in the present compound. Strain induced AFM to FM transition observed in La doped BiFeO₃ [28] and RMnO₃ (R = La–Lu) [29]. Reason for this transition is Jahn–Teller distortion which significantly enhances the ferromagnetism in the nearest-neighbor exchange interactions. In our case also we have observed a decrease in the second nearest neighbor distance which may increase the strength of exchange interactions.

To analyze more, the calculated nearest neighbor distance (NND) for different stress values are plotted in figure 2(b). At ambient, the first NND is found to be 2.96 Å (with four Ti and four Al atoms) and the value is same for Zr, Ti and Al atoms. In the case of Zr atom second NND is found to be 3.42 Å (with six Zr atoms). When we applied the bi-axial stress, third NND is observed for Zr which is not present at ambient. The first NND is not changed with positive stress values but it is found to increase with the application of negative stress. The values of second NND and third NND are found to decrease and increase with application of stress respectively. The number of atoms found with second and third NND are 4 and 2 respectively with the application of positive stress and the number is found to change as 2 and 4 with negative stress values.

We have calculated total and atom dependent magnetic moments at ambient FM case and under applied stress and are plotted in figure 2(c). At ambient FM case, the total magnetic moment of the system is found to be 1.906 μB with atom projected magnetic moments form Ti, Zr and Al are 1.440 μB, 0.242 μB and −0.019 μB respectively. Both Ti and Zr positively contributing to the total value but Al have a small negative value. The effect of negative stress is not much effective on the magnetic nature of the system as the magnetic moment values are almost same. But the scenario is not same with the applied positive stress. The total and atom dependent magnetic moments are found to decrease in nature with positive stress values. Particularly, the decreasing nature is more pronounced starting from 1.5% stress value. The magnetic moment, which is one of the physical properties of the solid will vanish with compression stress. Magnetism is completely vanished in Fe,
Co and Ni metals at pressures 18, 150 and 250 GPa respectively [30]. In the case of CaFe$_2$As$_2$ and BaFe$_2$As$_2$ compounds, pressure is a key parameter for vanishing the magnetic nature and phase change [31]. In the case of CsCl-type FeSe a transition from AFM phase to NM phase is observed with intermediate FM phase [32]. HCP Co is observed to become non-magnetic at a pressure of 180 Gpa with a series of electronic topological transitions (ETT) at different pressures [33].

Behavior of lattice parameter and crystal volume with applied stress are calculated and are plotted in figure 2(d). The values of $a = b$ are found to decrease with positive stress resulting an increase in the $c$ value, which causes for $c/a > 1$. The scenario is inverting with negative stress and resulting $c/a < 1$. The behavior of volume with stress are different with direction of the stress. Almost a linear increase in the crystal volume is observed with negative stress values. Application of positive stress is leading to non-monotonic behavior in the volume. Particularly, this behavior is starting at a stress value of 1.5%. Finally, it is ending with a flatted nature in the curve at 3.0% stress values. This nonmonotonic behavior in the crystal volume under compressive stress (particularly around 1.5% stress value) in the crystal may lead to electronic topological transitions (ETT). This can be seen in the Nb$_3$Al [34] and Nb$_3$Ga [35] based compounds experimentally and theoretically it is predicted because of ETT [36].

### 3.3. Electronic structure properties

To know the effect of strain/stress on the electronic structure details, total and atom dependent electronic density of states are calculated both at ambient and at strained/stressed conditions and are plotted in figure 3(a). At ambient, which is AFM ground state, overall contribution to the total density of states is highly dominated by Zr atom including at $E_F$. Ti atom dominated states are found only around 2 eV to 3 eV. Around 0.5 eV both atoms are contributing almost equally with a strong hybridization around the same energy range. At $E_F$, Zr-$d$ states are dominating more in compare with Ti-$d$ states. The value of total density of states at $E_F$ is found to be around 1.6 states/eV/f.u along with atom dependent values for Zr and Ti are around 0.87 and 0.5 states/eV/f.u.

The scenario is different with the application of strain/stress. The broad peak around 0.5 eV is found to be absent with stress and pseudo gap appeared in majority spin case in both stress cases. The states are moved towards the $E_F$, which causes the increase in the total density of states near $E_F$ with applied stress. The calculated values of total density of states at $E_F$ are found to be around 2.76 and 2.54 states/eV/f.u. for majority and minority spin cases respectively with 0.25% positive stress value and with 0.25% negative stress the values are 2.68 and 2.54 states/eV/f.u. respectively. At $E_F$ in stressed case, both Zr and Ti atoms are competing with each other in majority spin case but in minority spin case Zr atom is contributing more to the total density of states. From the total density of states with different stress values at the $E_F$, we have calculated electron spin polarization, $P = (N(E_F) \uparrow - N(E_F) \downarrow) / (N(E_F) \uparrow + N(E_F) \downarrow)$, where $N(E_F) \uparrow$ is total density of states at $E_F$ in majority spin case and $N(E_F) \downarrow$ is total density of states at $E_F$ in minority spin case. The calculated values of $P$ for 0.25%, 1%, 2% and 3% positive stress are 0.041, 0.104, 0.157 and 0.27 respectively. For 0.25%, 1%, 2% and 3% negative stress the P values are 0.027, 0.018, 0.024 and 0.06 respectively. From this it is observed that high electron spin polarization is observed with the application of positive stress in compare to negative stress. It is also observed that the polarization increases with increase in the stress values.

Electronic band structures of Zr$_2$TiAl for stress values $-0.25\%$ and $0.25\%$ are given in figures 3(b)–(e) for stable FM case. These calculations are performed with primitive cell to reduce the computational time and power. It is confirmed that, both majority and minority spins shows a metallic nature with the indication of bands which are crossing the $E_F$. The bands near the $E_F$ have a having mixed $d$-orbital nature from Zr and Ti atoms. The number of bands to cross $E_F$ are different with positive and negative stress. For positive stress it is one and two for majority and minority spin case respectively and it is inverting with negative stress.

Change in the electronic structure properties, in compare to ambient, is observed with the application of bi-axial strain/stress. Such difference of electronic structure with respect to the ambient case is maintained for the all the stress/strain values considered in the study. We have observed a phase transition in the present system. This indicate, the applied strain/stress may be highly effective on lattice part but not on the electronic structure part. To get more analysis regarding the structural modification, it is worth to calculate vibrational properties which will give more details about lattice part.

### 3.4. Vibrational properties

Dynamical stability of any system can be confirmed from the calculations of lattice vibrations. In the present case, a small positive/negative bi-axial stress cause for the ferromagnetic ground state in the present system with a phase change form fcc to bct. Here, we have performed phonon calculations with and without application of bi-axial stress in both FM and AFM cases. Calculated phonon dispersion along with total phonon density of states are plotted in figure 4. It is well known that the number of phonon modes will be equivalent to three times
Figure 3. (a) Total and partial density of states for ambient (middle plot) and stress cases (top and bottom one). Contribution of Al atom is not shown because of having very low states. Band structure for −0.25% stress (b), (c) and 0.25% stress (d), (e).
to the number of atoms in a primitive cell. In the present case we have four atoms in a primitive cell which will give rise to 12 phonon modes. Among them first 3 are acoustic and remaining 9 are optical modes.

The phonon band dispersion for FM and AFM are shown in figures 4(a) and (b) for ambient condition. A few important features to emerge. First, for both phases, there is no negative phonon branches, indicating that both phases are dynamically stable. Second, a clear phonon band gap of about 65 cm\(^{-1}\) ranging from 185 cm\(^{-1}\) to 250 cm\(^{-1}\) in FM case is observed and the same gap is found to reduced to a value of 50 cm\(^{-1}\) ranging from 200 cm\(^{-1}\) to 250 cm\(^{-1}\) in AFM phase. This is due to the frequency hardening at L point around 200 cm\(^{-1}\). Third, at X point, low frequency double degenerate acoustic mode around 20 cm\(^{-1}\) in FM case is found to become non-
degenerate with hardening in the frequency value in AFM case. We have observed visible shift of the middle frequency optical phonon branches and lower frequency acoustic branches between FM and AFM phases. This feature suggests a strong spin phonon coupling in this magnetic material at ambient case. The same behavior can be further understood from the total and partial phonon density of states. Partial phonon density of states of Zr, Ti and Al atoms for both FM and AFM phases are given in figure 5(a) (middle plot for ambient condition). The atomic mass of Zr, Ti and Al are 91.224 u, 47.867 u and 26.9815 u respectively. Due to larger mass of Zr atoms the modes below 150 cm\(^{-1}\) are dominated by Zr atom, the modes above 150 cm\(^{-1}\) to 200 cm\(^{-1}\) frequency region are dominated by Ti atoms which are having moderate mass and the vibrations of higher frequency optical modes consist of mainly lower mass of Al atom. From the same plots it is evident that the spin phonon coupling is more evident in middle frequency vibrational modes which are having heavily involved Ti atoms and partially involved Zr atoms.

A small bi-axial stress lead to the stability of the FM state with a structural phase transition. Phonon dispersion curves are plotted for both FM and AFM in figures 4(c) and (d) for 0.25% positive stress. For negative stress it is given in figures 4(e) and (f). For AFM case, with both positive and negative stress we have observed imaginary frequencies in phonon dispersion curves where no such imaginary frequencies appear for FM case. Some important points to highlight from these figures; first, except the higher frequency optical modes, all other vibrational modes are highly effected with the application of small bi-axial stress. Second, particularly in AFM phase, imaginary vibrational frequencies are observed at X, M and along Γ-M in acoustic modes with both
positive and negative stress values indicates the dynamical instability of the AFM phase with applied stress compared to ambient. Third, in FM case, both positive and negative stress phonon dispersion curves are having same nature which is also evident from the total and atom projected phonon density of states plots. We have tabulated the acoustic vibrational frequencies for non-magnetic cases at X and M high symmetry points in table 3 to know the stress effect on spin phonon coupling. In NM case, the first two acoustic modes are having higher imaginary values in compare to FM and AFM phases and the last acoustic mode is having higher positive values in compare to other phases. From this it is confirmed that the frequency hardening in the first two acoustic modes when we move from NM → AFM → FM but the last acoustic mode is behaving differently at different points. If we compare only FM and AFM magnetic phases, a large softening is observed in first two acoustic modes at X point with 0.25% stress, and with −0.25% stress it is observed only in first acoustic mode and the same softening is observed with both stress in first two acoustic modes at M point. This information confirms the large spin phonon coupling in the present system with bi-axial stress.

Table 3. Acoustic mode frequencies for both FM and AFM cases at 0.25% and −0.25% stress values. The frequency values are given in the units of cm⁻¹.

| Acoustic mode | 0.25% | −0.25% |
|---------------|-------|--------|
|               | FM    | AFM    | NM    | FM    | AFM    | NM    |
| at X point    |       |        |       |       |        |       |
| Eu            | 16.72 | −47.86 | −64.49| 25.63 | −42.65 | −62.54|
| Eu            | 19.27 | −9.80  | −59.71| 27.87 | 25.08  | −58.00|
| A2u           | 113.69| 101.31 | 122.18| 113.61| 103.94 | 121.94|
| at M point    |       |        |       |       |        |       |
| Eu            | 29.12 | −21.33 | −59.62| 11.56 | −35.06 | −63.63|
| Eu            | 29.12 | −21.33 | −59.62| 11.56 | −35.06 | −63.63|
| A2u           | 114.36| 126.97 | 122.92| 113.53| 111.37 | 122.32|

The analysis of total phonon density of states are very important in explaining the spin phonon coupling. The large peak in the high frequency optical region is found to be unchanged with the application of stress in compare to ambient, indicating that the effect of stress in higher frequency optical modes is negligible. This peak is due to vibrations of Al atom, which is not contributing to the magnetic nature in the present compound, is unaffected. The peaks in the middle and lower frequency regions are changing a lot with stress along with spin polarization. These peaks are mainly due to Ti and Zr atoms, which are contributing to the magnetic moments are showing different behavior in compare to ambient case. This illustrates the presence of spin phonon coupling in this material.

To know the behavior of total phonon density of states at higher stress values, we have plotted their values separately for FM and AFM cases at ambient and 1% strain in figure 5(b). It is observed that the over all behavior is almost same with FM case but in the case of AFM, we have observed a large softening in the middle frequency region peaks. This indicate AFM phase is more affected with applied stress in compare to FM phase. To compare FM and AFM phases, total phonon density of states plots are given separately for ambient, +1% and −1% stressed cases in figure 6. From this we can see a small hardening in the phonon frequency of AFM case at ambient, but in stressed case (1%) the values are almost same for both FM and AFM. A drastic change is observed in middle and lower frequency regions which is due to strong spin phonon coupling.

Finally, we will analyze the imaginary modes which are responsible for the instability in AFM phase with applied stress. These modes are observed at X, M points with positive stress, along with this we have continuous imaginary mode along Γ-M with negative stress. The atom dependent phonon density of states are given in the in-set of figure 5(a) (top and bottom plots). From this it is evident that Ti and Zr atoms have a large and equal contributions along with small contribution from Al atoms. The eigenvectors of these imaginary modes have been schematically shown in figures 7 and 8 for both positive and negative stress respectively. First mode at X point in 0.25% stress is because of in-plane vibrations of both Zr and Ti atoms perpendicular to each other in xy plane and remaining is only due to anti-parallel vibrations of Zr atoms. At M point, the imaginary modes are only due to Zr atoms. In −0.25% stressed case, we have only one imaginary mode at X which one is due to the Zr atoms but at M point we have two imaginary modes which are having contribution from all the atoms as shown in figures 8(b), (c).
4. Spin lattice coupling induced sharp AFM-FM transition

Figure 2(a) shows a very sharp AFM-FM (first order transition with respect to stress). Such behavior can be understood from the nature of coupling between the magnetism and the lattice. Following Glincuk et al [37], we can write the energy of the FM and AFM state as follows,
where $\mathbf{M}$ and $\mathbf{L}$ are the FM and AFM order parameters respectively, $\mathbf{u}$ can be considered as the displacement vector of a specific phonon mode which becomes unstable due to the application of the stress. The last term in both of the equation (1) represent the spin-lattice coupling, the constant $\lambda$ is same for both AFM and FM case as in $[37, 38]$. –ion, $E(\text{AFM}) < E(\text{FM})$, however as the stress is applied, the second term in the equation (1) can destabilize the AFM phase very fast if the magnitude of the displacement $|\mathbf{u}|$ cross a critical limit.

5. Conclusions

First principle electronic structure calculations for Zr$_2$TiAl are performed both at ambient and under bi-axial strain/stress. Total energy calculations are confirmed the FM ground state with all applied strain/stress along with a structural phase transition from fcc to bct. Band structure and density of states are analyzed in all strain/stress cases. The stability of FM state is also confirmed from the phonon dispersion calculations. The existence of imaginary frequencies at X and M points in AFM case confirms the spin phonon coupling in Zr$_2$TiAl.

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