IOP Conf. Series: Materials Science and Engineering **397** (2018) 012058 doi:10.1088/1757-899X/397/1/012058

Interfacial properties of Hg_2CuTi-type Heusler alloy Ti_2NiAl/GaAs(100) heterojunction

Yuanqiang Zhang [a,*], Lu Yang [a] and Xiude Yang [a]

[a] School of Physics and Electronic Science, Zunyi Normal College, Zunyi 563002, P. R. China

[*] Corresponding author: e-mail: 931019532@qq.com

Abstract. For Hg_2CuTi-type Inverse-Heusler alloy Ti_2NiAl/GaAs(100) tunnel heterojunction, the magnetism, density of states and spin polarization of atoms at the interface were investigated systematically based on the first-principle calculation within the density functional theory (DFT). The calculated results reveal that the interface states seriously destroy the structural half-metallicity and lead to the spin polarization less than 60%. Among all of calculational hetero-structures, only the heterojunction with TA-AT^{II} structure still retains nearly 60% spin polarization, which is expected for further application in Tunnel Magneto resistance (TMR) devices.

1. Introduction

Half-metal ferromagnets (HMFs), whose one sub-band across the Fermi level shows the metallicity while another sub-band is semiconducting with an energy gap, thus present a 100% spin-polarization at the Fermi level. For this reason, they have recently attracted more and more concerns applied for tunnel junction and spin injection in spintronics. Many HMFs, involving Fe_3O_4, CrO_2 have been also investigated and demonstrated [1]. Specially, in TMR system with a sandwich structure of ferromagnet/semiconductor/ferromagnet, HMFs are often served as ferromagnet layers for realizing the on/off effect controlled by an external electric field.

In TMR materials, Heusler alloy heterojunctions have been focused due to their high Curie temperature (CT), stable structures and well-matched mechanical properties to insulators or semiconductors, such as MgO and GaAs. Generally, Heusler alloys have four structural types: Full-Heusler, Half-Heusler, Hg_2CuTi-type Heusler and quaternary Heusler alloy. In these types, lots of studies have revealed that the narrower energy gap in bulk, spin-wave excitation, surface or interface defects can lead to serious TMR dropping with the increase of temperature [2-11]. To overcome such temperature dependence, many methods and techniques were devoted to seek more stable and wider band gap HMFs. In recent studies, Hg_2CuTi-type Heusler alloy, called as Inverse Heusler alloy yet, showed the more diversities of magnetism, excellent structural stability and wide band gap. In the past five years, some Ti-based Inverse-Heusler alloys, such as Ti_2CoAl, Ti_2NiAl, Ti_2CoGa etc were also confirmed with super half-metallic behaviors existing in the bulks [12-16]. Therefore, Hg_2CuTi-type Heusler alloy is deemed as a potential candidate, and it is quite necessary to deeply investigate Inverse Heusler alloy heterojunctions in TMR application.

In our work, by adopting the first-principle calculation within the DFT，the magnetism, density of states and spin-polarization of atoms in Ti_2NiAl/GaAs(100) hetero-interface were investigated comprehensively, and the potential structures with high spin polarization were also discussed.

Content from this work may be used under the terms of the Creative Commons Attribution 3.0 licence. Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI.
Published under licence by IOP Publishing Ltd

2. Calculation Details

Ti_2NiAl and GaAs bulk structures were first constructed based on their experimental lattice constants as the initial values. Hg_2CoTi-type Heusler alloy Ti_2NiAl has a F-43M space group, in which Ti atoms locate at (0,0,0) and (0.25,0.25,0.25) site, and Ni and Al atoms occupy (0.5,0.5,0.5) and (0.75,0.75,0.75) site respectively. After acquiring the lowest energy structure of optimization, the structure was cut into two natural terminal faces with 9 layers along [100] crystal orientation, corresponding to TiAl and TiNi terminal faces, respectively. For Ti_2NiAl, four different surfaces can be produced according to two different cutting ways per terminal face. As such, GaAs has the same number of different surfaces. Later, the two kinds of surfaces respectively in Ti_2NiAl and GaAs were combined to build a sufficiently large heterogeneous super-cell model, where both Ti_2NiAl and GaAs atomic layers are symmetric. In this way, the properties of the interface between Ti_2NiAl surface and GaAs(100) surface could be obtained after atomic relaxation. Finally, the eight different hetero-structures were built by the top site combinations between GaAs and Ti_2NiAl face atoms, as listed in Table 1. And their schematic diagrams of are depicted in Figure1.

Table 1. The different hetero-structures of Ti_2NiAl/GaAs(100) heterojunction by the top site combinations between GaAs and Ti_2NiAl.

Hetero-structure	TiAl face	Hetero-structure	TiNi face
TA-AT$^{\text{I}}$	Al -As	TN-AT$^{\text{I}}$	Ni -As
TA-GT$^{\text{I}}$	Al -Ga	TN-GT$^{\text{I}}$	Ni -Ga
TA-AT$^{\text{II}}$	Ti -As	TN-AT$^{\text{II}}$	Ti -As
TA-GT$^{\text{II}}$	Ti -Ga	TN-GT$^{\text{II}}$	Ti -Ga

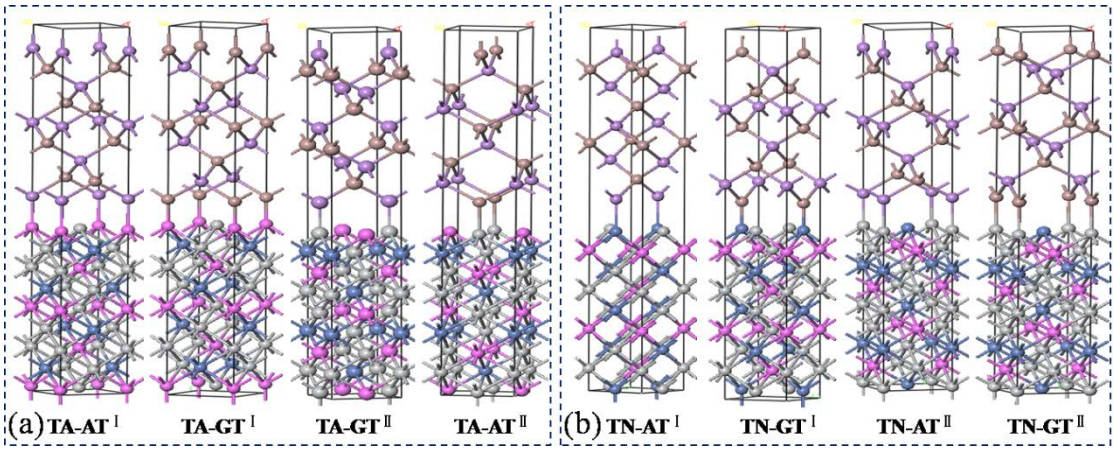


Figure1. The structural schematic diagrams in Ti_2NiAl/GaAs(100) heterojunction formed from different terminal faces. (a) TiAl face and (b) TiNi face. Among them, in lower 9 layers: the gray, blue and red ball is Ti, Ni and Al atom, respectively; while in upper 9 layers: the purple and yellow ball respectively represents As and Ga atom.

In this work, all calculations were performed by using VASP (Vienna ab initio Simulation Package) code within the DFT. And the PBE (Perdew-Bueke-Ernzerhof) correlation function within GGA (Generalized Gradient Approximation) [17-20] and the Vanderbilt-type urtrasoft psedopotentials [21,22] were adopted for dealing with the core-electrons interaction properly. During the initially optimized process for bulk structures, all alloys were firstly assumed to be ferromagnetic, and the spin polarization and a 7×7×7 grid of special k-points for Brillouin zone sampling were set. For self-consistent calculation, the energy convergence criterion of 1×10^{-6} eV/atom and the cutoff energy of 360 eV as well as the applied force less than 0.022eV/Å per atom were satisfied. As for the two-dimensional super-cell interface models, the grid precision of k-points for Brillouin zone was set to 7×7×1, and the other parameters were the same as bulk structure.

3. Results and Discussion

3.1 Magnetic Moments of Atoms in the Ti_2NiAl/GaAs Heterojunction Interfaces

Although each atom at Ti_2NiAl/GaAs(100) interface is different from the one in bulk under the action of other atoms, the impact of spin-orbit coupling on alloy is negligible. Therefore, only the magnetism variations of atoms at the interface were examined by calculating spin magnetic moments. For comparison, the magnetic moments of atoms both in bulk and four layers of different hetero-interfaces are summarized in Table 2 and 3. It can be seen that the magnetic moments of interfacial atoms seriously decreases in varying levels. In eight hetero-interfaces, magnetic moment of Ti atom with the highest value of 1.033μB in TN-GT^{I} and the minimum value of -0.038μB in TN-GT^{II} are discovered, which is 1.521μB in bulk. The discrepancy could be ascribed to the different interactions between Ti (or Al or Ni) atom and As (or Ga), relaxation processes and interface bonding behaviors, thus leading to an obvious decline of atom magnetism at the interfaces.

Table 2. The calculated atomic magnetic moment and total magnetic moment (TMM) in Ti_2NiAl bulk

Bulk	Ti (μ_B)	Ni (μ_B)	Al (μ_B)	TMM	SP value
Ti_2NiAl	1.521 0.003	0.171	0.985	2.7	3

Besides, It is also found that the farther away from the interface the atom is, the closer it is to the magnetic moment of the bulk, suggesting that the interface effect is reduced gradually as the number of atomic layers increases. So, the inner atoms are thought to be in a bulk and the interface impact can be ignored.

Table 3. The atomic magnetic moments of each layer in alloy Ti_2NiAl (100)/GaAs. HL and GL indicate Heusler alloy and GaAs layer respectively, the attached numbers of 1, 2,3 and 4 respectively represents the first, second, third and fourth layer under the interface, and the numerical value in bracket is corresponding to the magnetic moment of outer atom.

Hetero-structure	GL	HL1	HL2	HL3	HL4
TA-AT^{I}	As(-0.003)	Ti(0.011) Al(0.322)	Ti(0.328) Ni(0.234)	Ti(0.002) Al(0.126)	Ti(0.159) Ni(0.041)
TA-GT^{I}	Ga(-0.005)	Ti(-0.003) Al(0.898)	Ti(0.231) Ni(0.169)	Ti(-0.001) Al(0.087)	Ti(0.339) Ni(0.053)
TA-AT^{II}	As(-0.047)	Ti(-0.014) Al(0.602)	Ti(1.279) Ni(0.193)	Ti(0.002) Al(0.798)	Ti(1.279) Ni(0.307)
TA-GT^{II}	Ga(-0.006)	Ti(-0.002) Al(0.732)	Ti(0.191) Ni(0.164)	Ti(-0.001) Al(0.079)	Ti(0.247) Ni(0.047)
TN-AT^{I}	As(-0.010)	Ti(0.408) Ni(0.030)	Ti(-0.004) Al(0.132)	Ti(0.330) Ni(0.087)	Ti(0.000) Al(0.021)
TN-GT^{I}	Ga(0.000)	Ti(1.033) Ni(0.101)	Ti(-0.002) Al(0.238)	Ti(1.053) Ni(0.319)	Ti(0.012) Al(0.836)
TN-AT^{II}	As(0.017)	Ti(0.119) Ni(0.030)	Ti(0.001) Al(0.127)	Ti(0.154) Ni(0.069)	Ti(0.000) Al(0.040)
TN-GT^{II}	Ga(0.015)	Ti(-0.038) Ni(0.033)	Ti(0.001) Al(0.158)	Ti(0.305) Ni(0.095)	Ti(0.000) Al(0.019)

3.2 Electronic Behaviors on the Ti_2NiAl/GaAs Heterojunction Interfaces

To explore the interface effect on spin polarization of atoms and Ti_2NiAl/GaAs(100) structures, the total density of states (DOS) for each structure were calculated, respectively. Compared to the bulk with the half-metallicity, it is regrettable that none of half-metallic band-gap in all calculated hetero-structures of Ti_2NiAl/GaAs(100) is found due to the serious destruction deprived from the interface. The data show that the highest values of spin polarization is 55.77% in TA-AT^{II}, but the

other are less than 20%, which further demonstrates above results. Therefore, the TA-AT^{II} is considered as a relatively ideal structure discussed in details in following studies.

Next, the partial density of states (PDOS) of the four layer atoms in Ti_2NiAl (including TiNi and TiAl terminal faces) and the first layer atoms in GaAs at Ti_2NiAl/GaAs(100) interface are also calculated, as shown in Figs. 2 and 3. As the crystal's periodic field is cut off and the following re-hybridization happens, the interfacial magnetic atoms are mostly moved towards the high energy region. But in TA-AT^{II}, the opposite is true. Correspondingly, the spin polarization of atoms are boosted with the enhancement of exchange splitting. Hence, one preliminary conclusion is forecasted that the Ti_2NiAl/GaAs(100) heterjunction with TA-AT^{II} structure has a promising prospect in the TMR application.

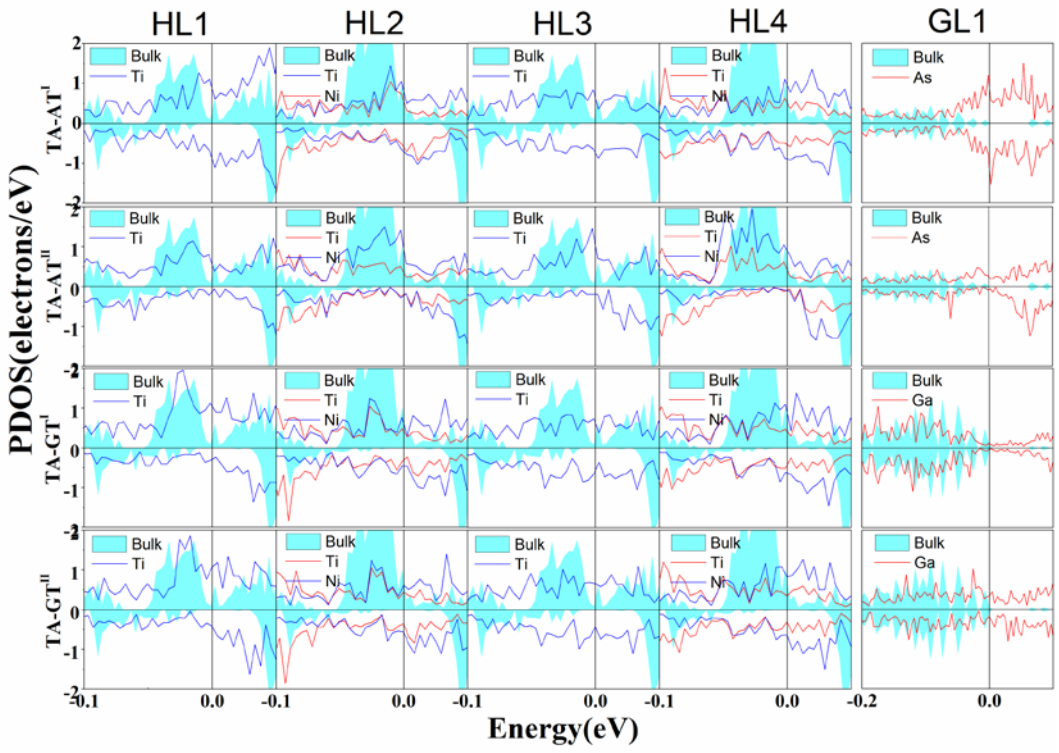


Figure 2. The PDOS of each layer atoms in alloy Ti_2NiAl/GaAs(100) hetero-structures from TiAl terminal face.

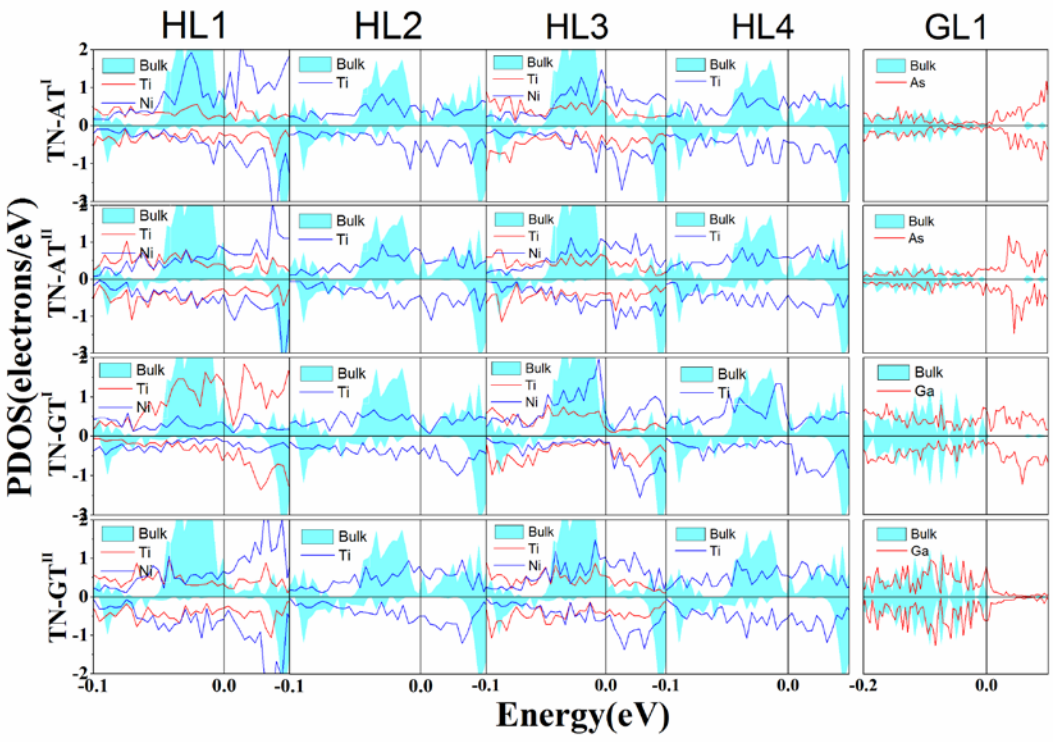


Figure 3. The PDOS of each layer atoms in alloy Ti_2NiAl/GaAs(100) hetero-structures from TiNi terminal face.

4. Conclusion

In summary, by adopting the first-principle calculation within DFT, the interaction, magnetism and spin polarization of atoms have been systematically investigated in Ti_2NiAl/GaAs(100) heterojunction. There are eight different hetero-structures by the top site combination between Ti_2NiAl and GaAs faces. The calculated results show that the interface effect has different levels of impact on the formed structures and consequently results in a serious degradation of the magnetism and half-metallicity. Among them, the TA-AT^{II} structure has the highest spin polarization of 55.77%, which is closest to the values in bulk. Therefore, it could be predicted that the Ti_2NiAl/GaAs(100) heterojunction with TA-AT^{II} structure deserves to be further exploited for TMR devices.

Acknowledgements

We gratefully acknowledge to the financial support from Natural Science Foundation of Technology Department (QKHJZ-LKZS[2014]10, QKHLHZ [2015]7020, Key Support Discipline ([2011]275) of Guizhou Province of China, and Key Laboratory and Scientific Research Foundation of Zunyi City (SSKH[2015]55).

References

[1] I.I. Zutic, J. Fabian, S.D. Sarma, Rev.Mod.Phys., 2004, 76: 323.
[2] D. Muri, D. School, H.C. Siegmann, E. Kay, Phys. Rev. Lett.,1988, 61: 758.
[3] A.H. MacDonld, T. Jungwwirth, M. Kasner, Phys.Lett. 1988, 81:705.
[4] C.H. Shang, J. Nowak, R. Jansen, J.S. Moodera, Phys.Rev.B., 1998, 58: r2917.
[5] C. Hoedequin, D. Ristoiu, L. Ranno, J. Pierre, Eur. Phys. J.B., 2006, 16: 287.
[6] C.N. Borca, T. Komesu, H.K. Jeong, P.A. Dowben, D. Ristoiu, Ch. Hordequin, J.P. Nozeres, J. Pierr, S. Stadier, Y.U. Idzerda, Phys. Rev. B., 2001, 64: 052409.
[7] J.J. Atterma, G.A.D. Wijs, R.A.D. Groot, J. Phys. Condens. Matter., 2007, 19: 315212.
[8] B. Wu, H.K. Yuan, A.L. Kuang, Y. Feng, H. Chen, J. Phys. D., 2011, 44: 405301.
[9] C. Supatutkul, S. Pramchu, A.P. Jaroenjittichai, Y. Laosiritaworn, Surf.Coat.Tech., 2016, 6: 364.

[10] F.B. Zheng, Q.F. Zhang, Q.Q. Meng, B.L. Wang, F.Q. Song, S. Yunoki, Q.H. Wang, Acta Mater. 2018, 59: 1607.
[11] B. Wu, H.K. Yuan, A.L. Kuang, Y. Feng, H. Chen, Appl.Surf.Sci.,2012, 258: 4945.
[12] G.D. Liu, X.F.Y. Dai, H.Y. Liu, J.L. Chen, Y.X. Li, G. Xiao, G.h. Wu, Phys. Rev. B., 2008,77: 014424.
[13] N. Kervan, S. Kervan, J. Phys. Chem. Solids., 2011, 72: 1358.
[14] N. Kervan, S. Kervan, Solid. State. Commun., 2011,151: 1162.
[15] L. Feng, C.C. Tang, S.J. Wang, W.C. He, J. Alloys Compd., 2011, 509: 5187.
[16] Y. Feng, B. Wu, H.K. Yuan, A.L. Kuang, H. Chen. J. Alloys Compd., 2013, 557: 202.
[17] J.P. Perdew, K. Burke, M. Ernzerhof, Phys.Rev.Lett., 1996, 77: 3865.
[18] W. Song, B. Wang, J.L. Wang, L. Fu, C.Y. Pu, X.M. Xu, Y.S. Zhu, C.Z. He, G.Q. Li, J. Clust. Sci., 2017, 28: 2575.
[19] J.P. Perdew, K. Burke, M. Ernzerhof, Phys.Rev.Lett., 1997, 78: 1396E.
[20] M. Rostami, Surf. Sci., 2018, 674: 103.
[21] D. Vanderbilt, Phys.Rev.B., 1990,41: 7892.
[22] Q.Y. Fan, Q. Wei, C.C. Chai, H.Y. Yan, M.G. Zhang, Z.X. Zhang, J.Q. Zhang, D.Y. Zhang, Indian Journal of Pure & Applied Physics, 2016, 54: 227.