The lattice distortion effect for zinc-blende CrAs and CrSb

2004 J. Phys.: Condens. Matter 16 S5815

(http://iopscience.iop.org/0953-8984/16/48/055)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **16** (2004) S5815–S5818 PII: S0953-8984(04)79430-8

The lattice distortion effect for zinc-blende CrAs and CrSb

Keita Yamana[1,3], Masaaki Geshi[1], Hidekazu Tsukamoto[1], Ichiro Uchida[1,4], Masafumi Shirai[2], Koichi Kusakabe[1] and Naoshi Suzuki[1]

[1] Graduate School of Engineering Science, Osaka University, Toyonaka, Osaka 560-8531, Japan
[2] Research Institute of Electrical Communication, Tohoku University, Sendai, 980-8577, Japan

Received 15 April 2004
Published 19 November 2004
Online at stacks.iop.org/JPhysCM/16/S5815
doi:10.1088/0953-8984/16/48/055

Abstract

We investigated the stability of the ferromagnetism of CrAs and CrSb in the zinc-blende structure against the lattice distortion, systematically. A calculation within the generalized gradient approximation using a full potential linearized augmented plane wave method was performed. We compared the ferromagnetic state and the antiferromagnetic state assuming tetragonal distortion with the lattice constants a and c changing independently and determined the spin polarization ratio in the ferromagnetic phase. The result shows that complete spin polarization (half-metallic ferromagnetism) remains stable even in the presence of large tetragonal distortion. On the other hand, our calculation shows that two monolayers of CrAs is enough to produce a half-metallic state in the CrAs/GaAs multilayer. Thus, the present result suggests that the half-metallic nature persists in various atomic-scale superlattices made of distorted CrAs or CrSb.

In recent years, there has been a great deal of research activity within a new discipline called 'spintronics' which aims at using the spins of electrons efficiently. To enhance the performance of future spintronics devices such as tunnelling magnetoresistance devices and spin field-effect transistors, it is desired to search for new materials having high spin polarization with ferromagnetism at room temperature. As prospective candidates, zinc-blende (zb-) CrAs and zb-CrSb have attracted the interest of many groups. Both zb-CrAs and zb-CrSb are newly predicted materials having completely spin-polarized band structure according to first-principles electronic structure calculations [1, 2] and they have now been synthesized successfully in experiments utilizing low temperature molecular-beam epitaxy [3, 4]. Experimentally, the ferromagnetic transition temperature is estimated to be above 400 K.

[3] Present address: Toyota Industries Corporation Technology Development Center, Dobu, 476-8606, Japan.
[4] Present address: NEC Micro Systems Ltd, Shiromi, Chuo-ku, Osaka 540-0001, Japan.

Unfortunately, the materials are not easy to obtain as bulk samples, since the thermodynamically stable structures of CrAs and CrSb are MnP type and NiAs type, respectively. In these experiments, zb-CrAs as well as zb-CrSb samples are grown as epilayers or thin films on the (001) surfaces of compound semiconductors. Thus, it is reasonable to assume that there is a certain amount of lattice distortion in the ferromagnetic substance caused by the substrate, although neither the lattice constants nor the spin polarization ratio is determined precisely in the experiments.

We performed first-principles calculations for zb-CrAs and zb-CrSb, where the lattice distortion is considered explicitly. The elastic properties of these compounds are estimated in the calculation. We show that half-metallic ferromagnetism remains stable even in the presence of a large tetragonal distortion. In later experiments, CrAs/GaAs multilayers on the atomic scale were successfully fabricated [5]. If we fabricate atomic-scale superlattices, a rather large lattice distortion is expected. The group of Shirai and the present group have performed several electronic structure calculations for atomic-scale superlattices made of CrAs and GaAs [6, 7]. By connecting the present result and findings on the superlattices, we conclude that the half-metallicity is rather stable in various atomic-scale superlattices.

First-principles calculations based on density functional theory (DFT) were performed. We utilized a full potential linearized augmented plane wave method. Calculations were done using the WIEN2k code [8]. For the distorted lattice, we fixed the muffin-tin (MT) radii to obtain systematic results. The MT radii are 2.08 au (Cr) and 2.12 au (As) for CrAs, while they are 2.19 (Cr) and 2.24 (Sb) for CrSb. The $R_{\mathrm{MT}}K_{\max}$ value is fixed at 8.00, where R_{MT} is a minimum MT radius and $K_{\max}$ is the maximum reciprocal lattice vector. We have used an angular momentum expansion up to $l_{\max} = 10$ inside the MT sphere. The criterion for the energy convergence is set to 0.1 μRyd. We have also checked the charge distance between the last two iterations. 484 k-points are taken in the reduced Brillouin zone. For the exchange–correlation functional we used both a local spin density approximation (LSDA) and a generalized gradient approximation (GGA) [9]. The lattice constants of zb-CrAs and zb-CrSb were determined. For zb-CrAs the lattice constants are 5.45 Å (LSDA) and 5.65 Å. For zb-CrSb these values are 5.95 Å (LSDA) and 6.15 Å. Though the values depend on the exchange–correlation energy functional (LSDA or GGA), on the whole, the tendency of the GGA results including the other properties as presented later is better than that of the LSDA. Thus, we choose the GGA results for discussing the physical nature of the materials.

We determined the lowest energy state within the DFT calculation by comparing the ferromagnetic state and the antiferromagnetic state. Within the calculated range of distortion, we always have a ferromagnetic state, although non-half-metallic ferromagnetism may appear.

The spin polarization ratios P for distorted Cr compounds are shown in figure 1. P is defined by $P = (D_\uparrow - D_\downarrow)/(D_\uparrow + D_\downarrow)$, where D_σ is the density of states for electrons with spin σ at the Fermi level. The calculation was done on a mesh of lattice constants a and c. For uniform compression of bulk structures, the spin polarization ratio decreases from the saturation value, when the lattice shrinks more than $\sim$1% from the equilibrium lattice constant for CrAs. The value is $\sim$6% for CrSb, showing strong stability of the half-metallic state of this compound against lattice distortion. When the lattice undergoes tetragonal distortion, the half-metallic state remains stable up to critical values of the lattice constants. The boundary line of the critical points on the (a, c) plane, where the half-metallic gap closes, is approximately given by a constant-volume line. If a thin film is made on a substrate, the lattice may distort, keeping the volume of the unit cell constant. Therefore, the half-metallicity should be preserved by the formation of a distorted lattice on a semiconductor surface.

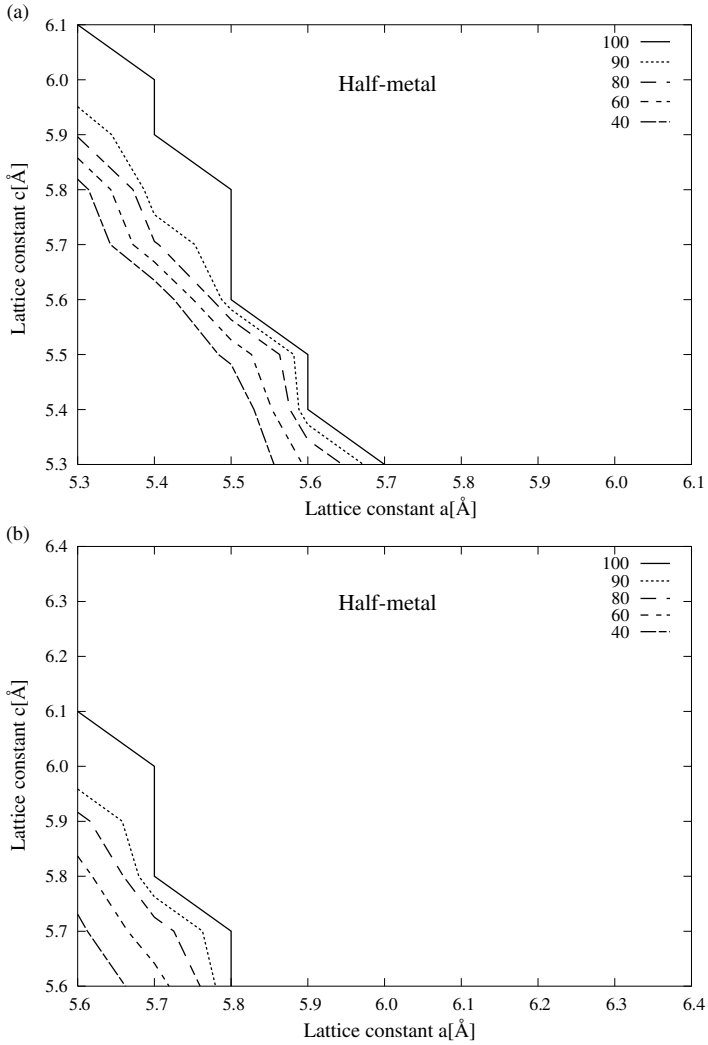

Figure 1. The spin polarization ratio P of (a) distorted zb-CrAs and (b) distorted zb-CrSb obtained by the DFT–GGA calculation. The figure shows a contour maps of P.

We have another quantity relating to the stability of the half-metal. The band gap of the minority spin is determined for the distorted lattices. In table 1, we summarize the values for zb-CrAs and zb-CrSb. The values are larger for zb-CrAs than for zb-CrSb.

The elastic properties are calculated and tabulated in table 2. The values obtained suggest that the elastic stiffnesses of zb-CrAs and zb-CrSb are almost the same as those of III–V semiconductors. When the superlattices are formed, both the ferromagnetic layer and the semiconducting layer may show lattice distortion.

To summarize our results, we have calculated spin polarization ratios of distorted lattices of zb-CrAs and zb-CrSb. The results indicate that the half-metallic state is rather stable against the lattice distortion. We can expect ferromagnetic behaviour in distorted films fabricated on various substrates. Our numerical data of the CrAs/GaAs multilayer [6, 7] suggest that the half-metallic state is stable in an atomic-scale layer, even if it is sandwiched by thick GaAs layers. 2 ML of CrAs is enough to produce a half-metallic state on the layer. Thus, the

Table 1. The band gap of the minority spin for (a) zb-CrAs and (b) zb-CrSb.

(a) zb-CrAs							
(a, c) (Å)	(5.8, 6.1)	(5.8, 5.8)	(5.8, 5.5)	(5.8, 5.3)	(5.3, 5.3)	(5.3, 5.7)	(5.3, 6.1)
E_g (eV)	1.85	1.94	1.79	1.62	1.22	1.21	1.15
(b) zb-CrSb							
(a, c) (Å)	(5.6, 5.6)	(5.6, 5.9)	(5.6, 6.2)				
E_g (eV)	1.08	1.01	0.93				

Table 2. The bulk modulus, B_0, its pressure derivative, B_0', and elastic constants, C_{11} and C_{12}, for zb-CrAs and zb-CrSb in the zinc-blende structure. The data for zb-GaAs determined by calculations and by experiments are shown for comparison.

	B_0 (GPa)	B_0'	C_{11}	C_{12}
zb-CrAs	69.8	4.81	82.9	78.3
zb-CrSb	49.1	5.01	44.1	40.7
zb-GaAs	60.0	4.35	101	43
zb-GaAs (exp.)	77 [10]	4.56 [11]	119 [12]	53.8 [12]
zb-GaSb (exp.)	56 [10]	4.75 [13]	88.34 [12]	40.23 [12]

thickness and lattice distortion do not have any great influence on half-metallic ferromagnetism in atomic-scale superlattices made of zb-CrAs or zb-CrSb.

Acknowledgments

This work was partly supported by a Grant-in-Aid from the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan (No 15GS0213), the MEXT Special Coordination Funds for Promoting Science and Technology (Nanospintronics Design and Realization), the 21st Century Centre of Excellence (COE) Programme 'Core Research and Advanced Education Centre for Materials Science and Nano-Engineering' supported by the Japan Society for the Promotion of Science (JSPS), the New Energy and Industrial Technology Development Organization (NEDO) under the Materials and Nanotechnology Programme and the Japan Science and Technology Corporation under the Research and Development Applying Advanced Computational Science and Technology Programme (ACT-JST).

References

[1] Shirai M 2001 *Physica* E **10** 143
[2] Shirai M 2003 *J. Appl. Phys.* **93** 6844
[3] Akinaga H, Manago T and Shirai M 2000 *Japan. J. Appl. Phys.* **39** L1118
[4] Zhao *et al* 2001 *Appl. Phys. Lett.* **79** 2776
[5] Mizuguchi M *et al* 2002 *J. Appl. Phys.* **91** 7917
[6] Nagao K, Shirai M and Miura Y 2004 *INTERMAG: 9th Joint Magnetism and Magnetic Materials (MMM)/ Int. Magnetic Conf.*; *J. Appl. Phys.* **95** 6518
[7] Geshi M *et al* 2004 *ACCMS-2: Asian Consortium on Computational Materials Science Proc.* to be submitted
[8] Blaha P, Schwarz K, Madsen G K H, Kvasnicka D and Luitz J 2001 *WIEN2k, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties* Karlheinz Schwarz, Techn. Universität Wien, Austria
[9] Perdew J P, Burke K and Ernzerhof M 1996 *Phys. Rev. Lett.* **77** 3865
[10] Cardona M and Harbeke G 1982 *Semiconductors. Physics of Group IV Elements and III–V Compounds* (*Landölt–Bornstein New Series,* Group III vol 17, Pt. a) ed K H Hellwege and O Madelung (Berlin: Springer)
[11] McSkimin H J *et al* 1967 *J. Appl. Phys.* **38** 2362
[12] Madelung O 1996 *Semiconductors—Basic data* 2nd revised edn (Berlin: Springer)
[13] McSkimin H J *et al* 1968 *J. Appl. Phys.* **39** 4127