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2002 J. Phys.: Condens. Matter 14 11007

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INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **14** (2002) 11007–11010 PII: S0953-8984(02)37301-6

Electronic properties of β-$FeSi_2$ under pressure

K Takarabe, R Teranishi, J Oinuma and Y Mori

Okayama University of Science, Ridai, Okayama 700-0005, Japan

Received 1 June 2002
Published 25 October 2002
Online at stacks.iop.org/JPhysCM/14/11007

Abstract
We have investigated for the first time the high-pressure optical absorption of β-$FeSi_2$ thin films (90 nm in thickness) prepared from Si/Fe multilayers on Si(001) with a template and SiO_2 capping. The pressure coefficient for the direct band gap of β-$FeSi_2$ is determined as 15.9 meV GPa^{-1}. This small coefficient is due to the negative deformation potential of the valence band maximum, and the large bulk modulus of β-$FeSi_2$.

1. Introduction

Iron disilicide, β-$FeSi_2$, has attracted much attention as a promising material for opto-electronic applications [1, 2]. β-$FeSi_2$ emits light at 1.55 μm (0.8 eV) suitable for SiO_2 optical fibre communications and epitaxial growth on Si is applicable. β-$FeSi_2$ is also known to be a Kankyo semiconductor (an ecologically friendly semiconductor) [3]. A well annealed thin-film sample shows a highest hole mobility of 13 000 cm^2 V^{-1} s^{-1} at 50 K, which exceeds the electron mobility [4]. Room temperature electroluminescence action has been already reported [5].

There are a growing number of studies on the basic properties of β-$FeSi_2$. For example, Filonov *et al* calculated the dielectric functions over a wide range of photon energies up to 5 eV, and compared these with ellipsometric experiments [6]. However, the nature of the band gap is still in dispute. Photoluminescence studies suggest that β-$FeSi_2$ is direct (for example [1]), but absorption studies suggest that it is indirect (for example [2]). Theoretical studies predict that the nature of the gap critically depends on the lattice strain of β-$FeSi_2$ [7–9].

Here, we performed a first-principles calculation of the optical properties of β-$FeSi_2$ focusing on the near-edge absorption coefficient, and report on the first high-pressure measurement of its absorption spectra up to 5 GPa. Note that some of the experimental work has been reported elsewhere [10].

2. Experiments

High-pressure optical spectra were measured by using a diamond anvil cell (DAC) in conjunction with a short-focal-length spectrometer attached to a 200 W tungsten lamp. Both the sample consisting of Si_{sub}(50 μm)/β-$FeSi_2$(0.09 μm)/SiO_2(0.1 μm) and the reference consisting of Si_{sub}(50 μm)/SiO_2(0.1 μm) were shaped into 200 × 200 μm^2 areas and put into a metal gasket with a 4:1 methanol–ethanol mixture as a pressure-transmitting medium. The

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Si substrate was thinned to 50 μm. The transmission measurements were performed for both the sample and the reference at various pressures, with the temperature held constant at room temperature. The direction of the incident light was parallel to the a-axis but not polarized.

3. Computational detail

A full-potential linearized augmented plane-wave (FLAPW) method implemented in the WIEN97 code was employed to calculate the electronic and optical properties of β-$FeSi_2$ [11]. The calculation was based on density-functional theory (DFT) and used a generalized gradient approximation (GGA). The basis set was expanded to about 2×10^3 plane waves outside the core region. A dense sampling up to 346 k-points in the irreducible Brillouin zone (BZ) was conducted for the self-consistent cycle.

The crystal structure was base-centred orthorhombic ($Cmca$) and the primitive unit cell consisted of 8 Fe atoms and 16 Si atoms. The bulk lattice constants and internal positions for each atom were attained from previous experiments [12].

4. Results and discussion

4.1. Band structure under pressure

The calculated band structure is shown in figure 1. The valence band maximum (VBM) is at Y, $(2\pi/a, 0, 0)$, and is more than 0.1 eV higher than the local maximum along the $Z\Gamma(\Lambda)$ direction. The conduction band minimum (CBM) is along the $Z\Gamma(\Lambda)$ direction. Thus, the Y–Λ indirect gap is 0.67 eV and the direct gap at the Y point is 0.73 eV. The next direct band gap along the $Z\Gamma(\Lambda)$ direction is 0.81 eV. On the other hand, the experimental direct band gap is 0.873 eV at room temperature as discussed later. The theoretical band gap is 0.143 eV lower than the experimental result. It is well known that the DFT theory underestimates the band gap. Comparing this with various different first-principles calculations [7–9, 13, 14], the topology near the gap is the same except for the quantitative difference in energy. This topology is in contrast to that of Filonov *et al* [6] who reported that the VBM was along the Λ direction and the Y point was lower than the VBM. It is also in contrast with the result of Christensen, who suggested that the VBM was at the Γ point [15].

Figure 1 shows the band structure under compression with $V/V_0 = 0.983$ together with that at an ambient pressure. The VBM is taken as the reference, so the relative change of the band gap can be seen. There is no obvious change in the dispersion of the valence band and the conduction band except for the uniformly upward shift in energy. This contrasts sharply with the band-gap pressure coefficients in common semiconductors such as Si and GaAs; in particular the Γ and X conduction band edges are opposite in sign.

4.2. High-pressure absorption experiment

The absorption spectra at various pressures are shown in figure 2. The absorption edge is known to be around 0.8 eV, and the change in the slopes is seen at around 0.9 eV at ambient pressure. From the calculated band structure in figure 1, the first absorption edge is indirect and the second is direct. To conclude that the first edge is indirect, it is necessary to observe a phonon replica of the absorption spectra in a similar way to in common semiconductors. However, the sample here was too thin to observe the absorption coefficient below the indirect gap, where the interference fringes mask the detail of the absorption spectra. On the other hand, a very similar result was reported by Henrion *et al* [16] for MBE grown film of 750 nm thickness on Si. This is about eight times thicker than our sample. Henrion *et al* claimed that they observed a one-phonon emission and absorption spectrum, and reported that the indirect edge was at 0.75 eV and the direct edge was at 0.87 eV. Although the measurement was limited to photon

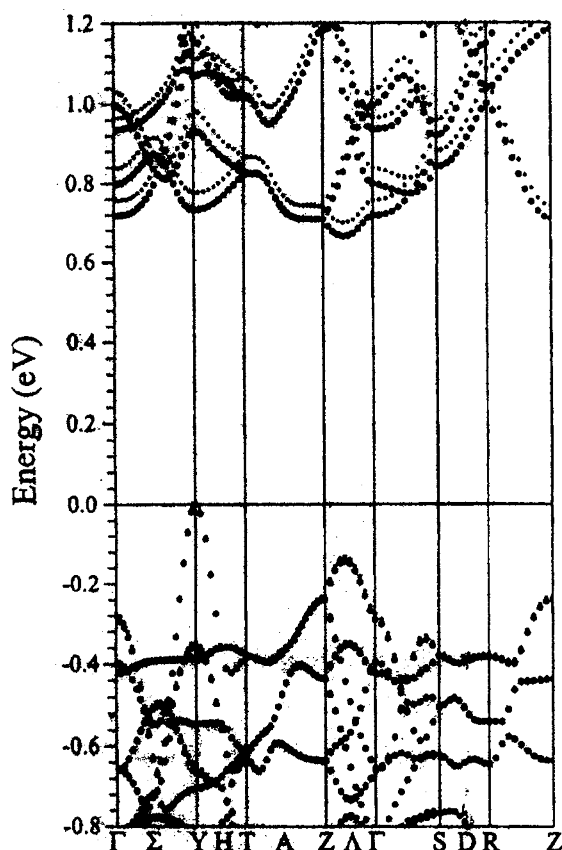

Figure 1. Band structures with and without compression along high-symmetry axes. The VBM at the Y point is taken as the reference energy.

energy up to 0.95 eV, the result of Henrion *et al* shows that the energy difference between the indirect and direct edges is about 0.12 eV. This separation deviates by about 0.06 eV from the calculated band structure. On increasing pressure, the absorption spectra move in parallel to higher energies up to 5 GPa. There is no observable change in the spectral shape like that seen in GaAs when crossing from the direct to the indirect gap.

The evaluated linear pressure coefficient of the direct band gap is 15.9 meV GPa^{-1}. The pressure coefficient of the Γ direct gap is, for example, 108 meV GPa^{-1} for GaAs [17]. Consequently, that of β-$FeSi_2$ is 6.8 times smaller than that of GaAs. The bulk modulus of β-$FeSi_2$ is 180–200 GPa, 2.4–2.7 times larger than the value 75 GPa for GaAs [14, 15, 18]. This inherent hardness of β-$FeSi_2$ can account for only about 40% of the smallness of the pressure coefficient of the direct band gap compared to GaAs. On the other hand, the band-gap deformation potential of β-$FeSi_2$ at the Y point is calculated to be -2.4 eV from three different volumes of $V/V_0 = 1.0$, 0.983, and 0.967. The magnitude of this theoretical deformation potential is again 3.5 times smaller than the value -8.33 eV for GaAs [19]. The main reason for this difference is that the absolute deformation potential of the VBM in β-$FeSi_2$ is negative from our calculation, which shows that the VBM shifts to higher energy with increasing pressure. This behaviour is in contrast to that for GaAs and other common semiconductors, for which the deformation potential is opposite in sign, and, therefore, the VBM is lowered in energy. The chemical picture for this behaviour in common semiconductors is that the VBM is the bonding state.

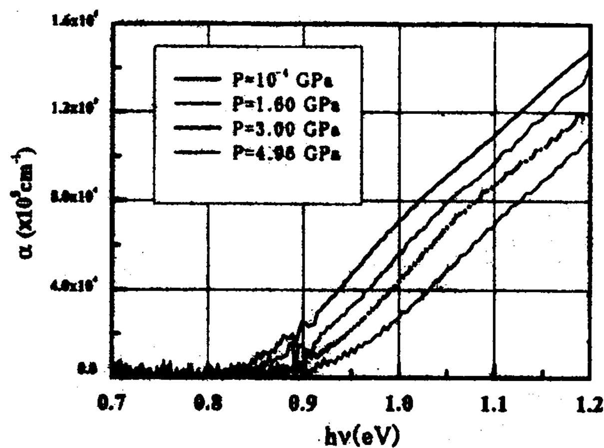

Figure 2. Experimental absorption spectra at various pressures.

5. Conclusions

A high-pressure optical absorption experiment on epitaxially grown β-$FeSi_2$ on a Si(001) substrate and first-principles FLAPW calculations of the band structure and optical absorption coefficients have been reported. By combining the experimental and theoretical absorption coefficients, the band gap of relaxed epitaxially grown β-$FeSi_2$ on Si(001) substrate is shown to be indirect with a direct gap lying several tenths of a millielectron volt higher. The indirect transition occurs along the $Z\Gamma(\Lambda)$ direction and the direct transition occurs at the Y point. The pressure coefficient of the direct band gap is determined as 15.9 meV GPa^{-1}. Two possible reasons for this small pressure coefficient compared with those common semiconductors are the negative absolute deformation potential of the VBM, and the large bulk modulus of β-$FeSi_2$.

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