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On the band diagram of Mg_2Si/Si heterojunction as deduced from optical constants dispersions

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Abstract

The optical constant dispersions of ion-beam-synthesized Mg_2Si phase in Si matrix are obtained from the transmittance and reflectance spectra. Two types of samples are studied – one of them with Mg_2Si phase embedded in *n*-type (100)Si and the other with Mg_2Si phase embedded in *p*-type (100)Si. The formation of the phase is proved by Raman scattering and infrared transmittance measurements. From the interpretation of the optical constant dispersions, the energies of the transitions nearby the material band edge are determined. As a result the band diagram of the heterojunction Mg_2Si/Si is obtained. The results about the Mg_2Si band gap value are compared with the theoretically predicted and experimentally determined ones. The value of the conduction band offsets of Mg_2Si and Si is not reported by now.
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1. Introduction

The compound Mg_2Si is among the few semiconducting silicides. The semi-conducting silicides are compatible with the well-developed silicon technology and provide prospects for silicon-based integration. Possible applications are also in opto-electronic, thermoelectricity and photovoltaic. On the other hand, due to the abundance of the constituting elements in nature and non-toxicity, the semi-conducting silicides have attracted much interest as cheap and environment friendly materials.

The fundamental properties of Mg_2Si bulk crystals are investigated both theoretically and experimentally [1–9]. The theoretical calculations of the energy band structure predict an indirect band gap with values varying from 0.118 to 0.7 eV. The optical investigations give the values in the interval from 0.60 to 0.66 eV [6] and the value, determined from the electroconductivity temperature dependence, is 0.78 eV at 0 K [5].

The optical properties of Mg_2Si thin films and low-dimensional structures are purely studied due to the difficulties in the growth. The thin films formation appears to be complicated because of the low condensation coefficient of magnesium as well as of the limited Mg_2Si films thickness, due to the barrier behavior of Mg_2Si [10]. Mahan et al. [11] succeeded in preparing stoichiometric Mg_2Si films, textured in (111) direction, by molecular-beam epitaxy using co-deposition of magnesium and silicon with a magnesium-rich flux. From the investigation of the transmittance and reflectance spectra of these films, Mahan et al. [11] determine the value of the first indirect interband transition to be 0.74 eV. Two direct interband transitions at 0.83 and 0.99 eV are determined also. Solid-phase growth technique with preliminary formation of templates is used by Galkin et al. [10] to prepare continuous Mg_2Si films with a thickness of the order of 20 nm on Si(111) substrates. Galkin et al. [10] report the value 0.75 eV for the first indirect transition and the values 0.90–0.95 eV and 1.03–1.05 eV for the higher energy direct transitions.

The very low condensation coefficient of magnesium as well as the limited Mg_2Si films thickness due to the barrier behavior of Mg_2Si can be avoided using the ion-beam synthesis (IBS) [12]. In this work the transmittance and reflectance spectra of samples, representing silicon matrix with Mg_2Si phase, embedded in it in the form of layers and precipitates, are studied. From the interpretation of the optical constant dispersions, the following energies are determined: (i) the conduction band (CB)

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offset of the heterojunction Mg_2Si/Si; (ii) the transition energies in the vicinity of the Mg_2Si band gap; (iii) an additional energy, attributed to the transition from the Mg_2Si valence band (VB) top to the Si CB bottom at the interface.

2. Experiment

2.1. Samples preparation

The samples are prepared by IBS, followed by rapid thermal annealing in vacuum 6.65×10^{-3} Pa. Mg ions with dose 4×10^{17} cm^{-2} are implanted with two different energies: $\mathbf{E}_i$=40 keV into *n*-type (100)Si substrates with ρ=4.5–5 Ω cm and $\mathbf{E}_i$=60 keV into *p*-type of (100)Si substrates with ρ=2.5–5 Ω cm. In Fig. 1 the Mg implantation profiles of the samples, implanted with the two different energies, are given.

The concentration profiles are simulated by the SRIM (Stopping and Range of Ions in Matter) program. It is seen that the Mg concentration is lower than the Mg_2Si stoichiometric one (66.66 at.% Mg) in the whole implantation depth. The higher implantation energy leads to lower Mg concentration and larger implantation depth.

During the implantation, in order to avoid the substrate amorphization, the samples are heated to a temperature of about 230 °C by means of the incident ion beam. After the implantation the samples are annealed at the same temperature, 500 °C. Samples, implanted with both energies, are annealed for different times. In the samples notation the first figure stands for the implantation energy (4 means $\mathbf{E}_i$=40 keV and 7 means $\mathbf{E}_i$=60 keV) and the second one – for the annealing time t_a (0 means unannealed sample, 1 – annealed for 30 s, 2 – for 60 s, 3 – for 300 s).

2.2. Samples characterization

The formation of the Mg_2Si phase is proved by IR transmittance (*T*) and Raman scattering. In Fig. 2 the IR spectra of the samples, taken by BOHMEM Fourier spectrometer, are shown in the wave number range from 200 to 400 cm^{-1}. The well-observed minimum in the IR transmittance spectra of all the samples is positioned at 272 cm^{-1}. The wave number position of the minimum coincides fairly well with the one obtained both by theoretical calculations and experimental investigations [13,14] of bulk material and can be attributed to the infrared-active F_{1u} mode of the Mg_2Si phase.

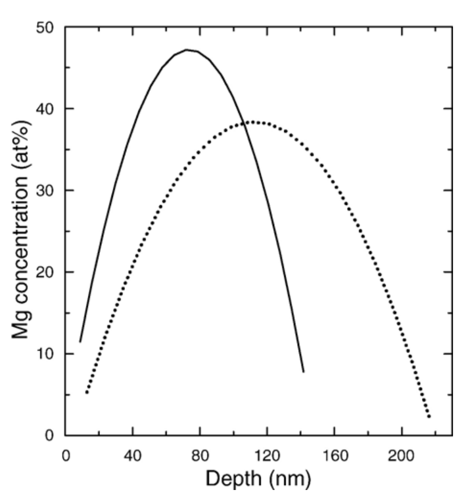

Fig. 1. Mg implantation profiles at two different energies: 40 keV (full line) and 60 keV (dotted line) and the same doze of the implanted Mg ions (4×10^{17} cm^{-2}). The profiles are simulated by SRIM.

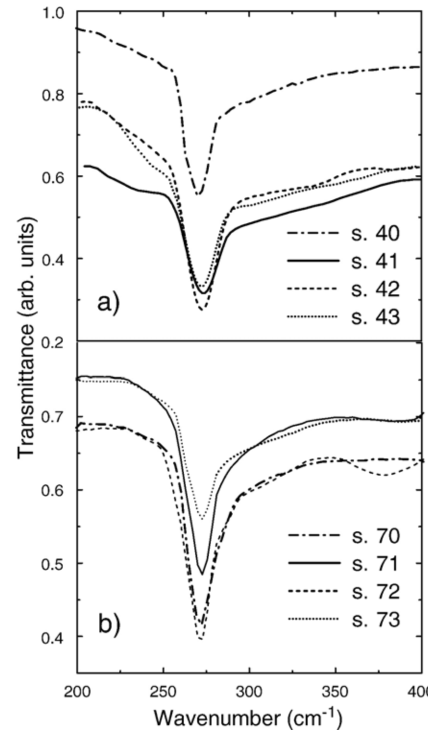

Fig. 2. IR transmittance spectra of the samples, prepared with the same doze of the implanted Mg ions (4×10^{17} cm^{-2}) and with two different energies: (a) $\mathbf{E}_i$=40 keV and (b) $\mathbf{E}_i$=60 keV. The samples are annealed for different times as denoted in the figure – s. 40 and s. 70 are unannealed, s. 41 and s. 71 are annealed for 30 s, s. 42 and s. 72 – for 60 s, and s. 43 and s. 73 – for 300 s.

The unpolarized spectra of the Raman scattering, shown in Fig. 3, are measured with SPEX 1403 double spectrometer equipped with photomultiplier, working in a photon counting mode. The Ar^+ laser line with wavelength 488 nm was used for excitation. The spectra were taken with spatial slit width 4 cm^{-1} and accumulated with frequency 1 cm^{-1}. Two peaks are detected in the spectra of both types of samples, the main one – at wave number 256 cm^{-1} and the second – at 345 cm^{-1}. An additional strong peak at 516 cm^{-1} is seen only in the spectra, produced with $\mathbf{E}_i$=60 keV. The main structure, seen in our experimental Raman spectra at wave number 256 cm^{-1}, coincides well with the value, cited for the first-order Raman-allowed F_{2g} phonon mode in bulk materials [13–18]. A feature of the Raman scattering in the material is the scattering by Fröhlich-interaction-induced otherwise Raman-inactive longitudinal optic (LO) F_{1u} mode [18,19], resulting in a sharp peak at wave number 348 cm^{-1}. The sharp peak at 345 cm^{-1} has obviously to be attributed to the F_{1u} (LO) mode. In the spectra

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