

# Optical properties of thin-film magnesium silicide prepared by electrochemical process

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Received 25 November 2005; received in revised form 27 February 2007; accepted 27 February 2007

Available online 4 March 2007

## Abstract

We report the optical properties of a thin-film  $\text{Mg}_2\text{Si}$ , which was successfully prepared as a continuous and homogeneous polycrystalline phase on a Si(1 0 0) face by an electrochemical process with a thickness greater than  $10 \mu\text{m}$ . The growth rate achieved in the process was the order of  $10 \mu\text{m/h}$ . Optical absorption coefficient spectra obtained at room temperature exhibited an absorption edge at around  $0.8 \text{ eV}$ . Assignments of the peaks in the spectra to the optical transitions were based on using conventional reports. The absorption bands at  $1.90$  and  $2.63 \text{ eV}$  are consistent with the reported direct transitions in the reflectance measurements for single crystals and the results of band calculations. The absorption at the band edge, which is claimed to be an indirect transition from the calculations, contains a substantial direct absorption.

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**Keywords:** Silicide semiconductors; Optical properties; Photovoltaic-cell materials; Electrochemical process; Magnesium silicide

## 1. Introduction

Silicide semiconductors have attracted intensive studies for the last few decades [1] because of their advantages over conventional silicon and compound semiconductors. Many of the silicides have large absorption coefficients mainly because they have a direct bandgap in the thin-film form [1–4]. This optical property, which is favorable for use as a solar photovoltaic-cell material, is in good contrast to that of the c-Si, which has an indirect bandgap. Additionally, the absorption edge of silicon does not necessarily locate at the right energy position for the maximum efficiency. The bandgap energy of the metal silicides can range from the infrared (Ba, Mg, Fe) to visible (Ca) region [1,4–6] by choosing the metal elements and phase of the compounds, without less-common and/or environmentally less-friendly elements in many of the compound semiconductors. Besides, they are free from the optically induced conductivity decrease which a-Si:H suffers [7]. Nevertheless, it is often very difficult or needs long time to achieve the growth of their continuous film layer of a few micrometers, which is characteristic of the photovoltaic-cell materials, by deposition and/or

reaction from the gas-phase [8–14] even though it is relatively easily obtained in the powder form as a starting material for thermoelectric devices [15].

In the present study, we report the optical properties of a thin film comprised of a continuous and homogeneous polycrystalline  $\text{Mg}_2\text{Si}$  layer, which is  $\sim 10 \mu\text{m}$  thick on a Si plate with the growth rate on the order of  $10 \mu\text{m/h}$ . This synthesis has been achieved by an electrochemical technique using a LiCl–KCl molten salt. For the film of this compound on the Si plate, there have been reported those on the order of  $0.1 \mu\text{m}$  by deposition from gas-phase [16–20], or those with a thickness of  $200 \mu\text{m}$  through 72-h reaction in a Mg vapor [13,14].

## 2. Experimental

The thin film samples were prepared on a Si(1 0 0) face of an Si wafer (Nilaco Co. Ltd.) by potentiostatic electrodeposition in a LiCl–KCl eutectic melt at  $723 \text{ K}$ . A  $15 \text{ mm} \times 5 \text{ mm}$  electrode area was used. Magnesium ions were supplied as  $\text{MgCl}_2(0.1 \text{ mol}\%)$  in the melt. As we see in Fig. 1, the formation of a continuous and homogeneous film with a thickness of  $10 \mu\text{m}$  was achieved by potentiostatic electrolysis at  $0.8 \text{ V}$  (versus  $\text{Li}^+/\text{Li}$ ) for 1 h. Only the  $\text{Mg}_2\text{Si}$  phase, other than the Si substrate, was confirmed in the XRD analysis as shown in Fig. 2. The diffraction peaks for the compound became even

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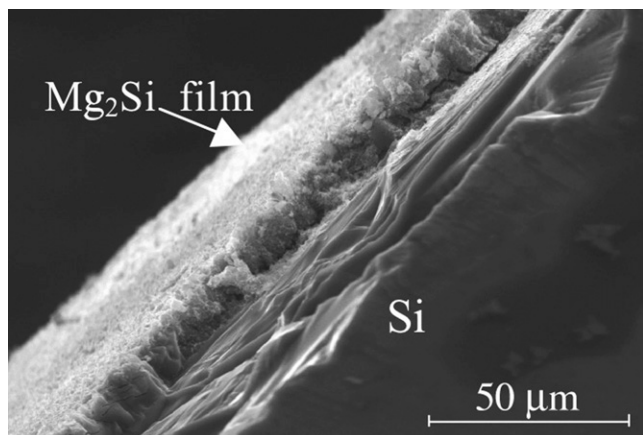


Fig. 1. Cross-section SEM image of the cleaved sample prepared by potentiostatic electrolysis at 0.8 V for 1 h on the Si(100) face [21].

more distinctive than those electrolyzed at 0.8 V for 3 h. Details of this novel electrochemical process for silicide formation and the results of the quantitative elemental analysis and electrochemical analysis are to be reported by Goto et al. [21].

The reflectance was measured by a spectrometer. The Kubelka–Munk function [22]:

$$\frac{\alpha}{s} = \frac{(1 - R_d)^2}{2R_d} \quad (1)$$

was used to convert the diffuse reflectance,  $R_d$ , into an optical absorption coefficient,  $\alpha$ . The scattering coefficient,  $s$ , is less dependent on energy at least near the bandgap where the absorption intensity is low and the peak positions never change.

### 3. Results

The diffuse reflectance spectra is presented in Fig. 3. The calculated absorption coefficient from Eq. 1 using the spectra in Fig. 3 is given in Fig. 4.

As has been demonstrated by Mahan et al. [18] for the film with a thickness of  $\sim 0.08 \mu\text{m}$ , a large absorption is observed at 0.8–1.2 eV, which is absent in Si. This feature should be important for photovoltaic-cell materials. Several optical transition peaks are also observed at 1.90, 2.63 and 3.02 eV.

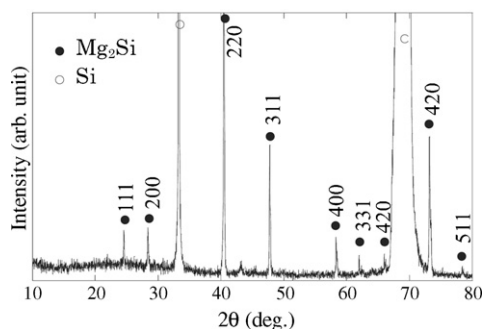


Fig. 2. XRD pattern for the sample prepared by potentiostatic electrolysis at 0.8 V for 1 h on the Si(100) face [21].

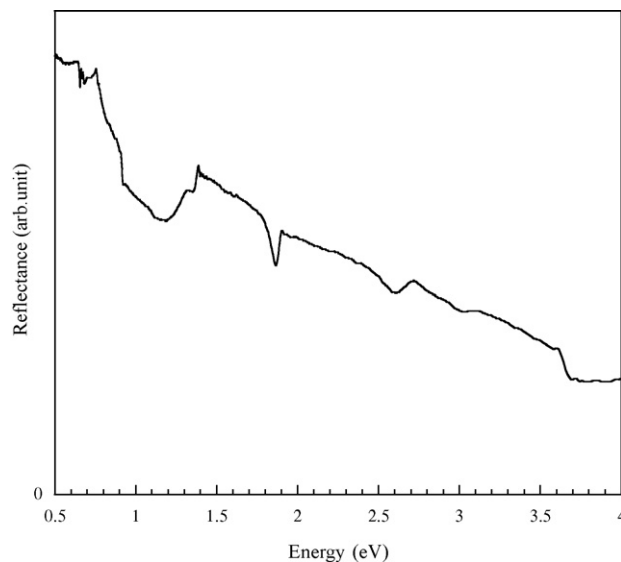


Fig. 3. Diffuse reflectance spectra at room temperature for  $\text{Mg}_2\text{Si}$  on the Si(100) face.

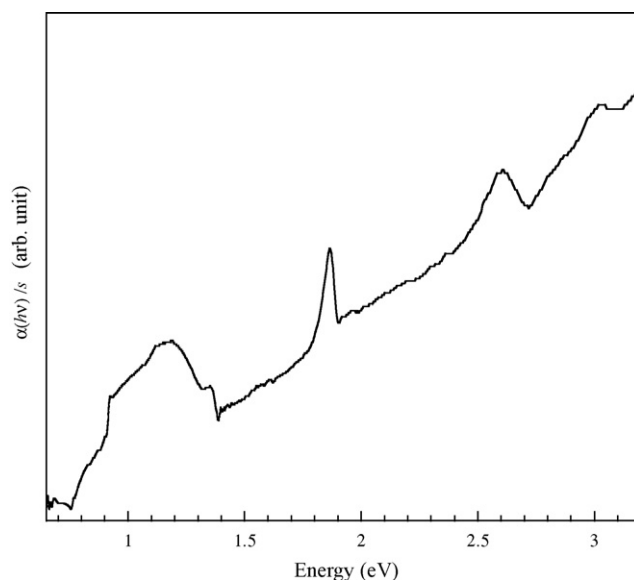


Fig. 4. Optical absorption coefficient at room temperature for  $\text{Mg}_2\text{Si}$  on the Si(100) face converted from the diffuse reflectance.

### 4. Discussion

The plots of  $(\alpha h\nu/s)^2$  and  $(\alpha h\nu/s)^{1/2}$  versus energy are presented in Figs. 5 and 6 for the determination of the absorption edge. These plots suggest that the direct absorption edge is located at 0.77 eV and the indirect absorption band lies just above that at 0.83–0.84 eV. According to a band calculation [23], this compound is expected to have an indirect bandgap. The indirect absorption at the band edge was indeed observed at 0.74 eV in the report for a film [18] and also at  $\sim 0.8$  eV for a single crystal sample at 300 K [24]. Nevertheless, the former, a film sample of  $\sim 0.08 \mu\text{m}$  thickness, also exhibited a transition just above the band edge at 0.83 eV. Mahan et al. [18] assign this absorption,

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