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Optical characterization of boron-doped nanocrystalline Si:H thin films

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Abstract

We report on the optical properties of boron-doped hydrogenated nanocrystalline silicon (nc-Si:H) thin films grown on glass substrates by plasma-enhanced chemical vapor deposition (PECVD), using X-ray diffraction (XRD), Raman scattering, and optical transmission measurements at room temperature. Wavelength-dependent optical constants (refractive index and extinction coefficient) are deduced from the optical transmission spectra by the well-known Tauc–Lorentz (TL) model with an empirical modification, instead of the conventional envelope method. The refractive-index behavior (magnitude and dispersion) below the interband absorption edge can be well described by the one-oscillator Wemple–DiDomenico model, which also reveals structural information of these nc-Si:H samples. The extinction coefficients are very close to those obtained independently by the Forouhi–Bloomer (FB) model. New physical significance implicit within the TL model has been tentatively discussed on the basis of the refractive-index results of the B-doped nc-Si:H in this work, and intrinsic nc-Si:H as well as many other Si-related materials in the literature.
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1. Introduction

During the last few years, hydrogenated nanocrystalline silicon (nc-Si:H) thin films have received great attention due to their potential applications in optoelectronic devices such as single electron transistors, solar cells, and thin film transistors. nc-Si:H thin films are two-phase-mixed materials where silicon nanocrystals are embedded in an amorphous silicon matrix [1]. Several deposition techniques have been established to prepare nc-Si:H thin films, including plasma-enhanced chemical vapor deposition (PECVD), hot wire chemical vapor deposition, and radio-frequency (rf) magnetron sputtering, among which PECVD appears to be a promising deposition method for large-area thin film technology and has been employed for industrial applications [2]. *p*-type nc-Si:H or hydrogenated microcrystalline silicon thin films, whose electrical properties have been extensively studied [2–4], present an attractive alternative in applications to optoelectronic devices because of their greater doping efficiency, higher electrical conductivity, higher mobility, etc., as compared with *p*-type hydrogenated amorphous silicon (*a*-Si:H). A detailed knowledge of these electrical properties as well as the optical properties in nc-Si:H is of technological importance from the viewpoints of both fundamental physics and future applications. However, little information about optical constants of the *p*-type (such as doped by boron) nc-Si:H thin films is available in the literature so far, although some relevant results were reported for the intrinsic ones [5–8].

As is well known, wavelength-dependent optical constants (refractive index and extinction coefficient) of semiconductors can be extracted from optical transmission/reflection and spectroscopic ellipsometry (SE) data, using various empirical formulas [9], effective-medium theories [8,10], or dielectric function models (DFMs) [11–13]. In general, the DFMs are preferable in spectral simulation due to not only their Kramers–Kronig consistency, but also their convenient analytic representation of the semiconductor dielectric responses. Several DFMs have been established

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and widely used including the well-known Tauc–Lorentz (TL) model [11], Forouhi–Bloomer (FB) model [12], and Adachi model [13], among which the former two models with the least fitting parameters (i.e., only five parameters) were originally proposed for amorphous materials and subsequently used in crystallized or nanocrystalline semiconductors [5–7,14]. As far as the TL and FB models are concerned, although the latter shows superiority over the former in the investigation of thermal effects on optical band gaps as well as optical constants in the interband region of *p*-type nc-Si:H [15], it is an open question that which model is more suitable to describe the relatively true spectral behavior of optical constants, particularly the refractive-index behavior below the interband absorption edge of these doped materials, in which the refractive index values can be influenced by possible free carrier absorption. Furthermore, the TL model [11], which was proposed empirically by Jellison and Modine in 1996, can overcome some inherent shortcomings within the FB model proposed theoretically 10 years earlier and has almost become the most popular one in the world; nevertheless, its implicit physical significance is not yet fully understood.

The purpose of this paper is twofold: (i) to report the relatively reliable spectral dependence of refractive index as well as that of extinction coefficient extracted from room-temperature optical transmission spectra of boron-doped nc-Si:H thin films, using the TL model with an empirical modification based on the comparison between the TL and FB models, and (ii) to tentatively elucidate new physical significance implicit within the TL model.

2. Experimental details

The two typical *p*-type nc-Si:H thin films investigated were prepared in a 60-W rf (13.56 MHz) capacitive coupled PECVD system from silane (SiH_4) and hydrogen (H_2). Diborane (B_2H_6) was used as dopant gas. The hydrogen dilution ratios (H_2/SiH_4) were 62.5 and 97.1 for samples A1 and A2, respectively, with diborane doping ratio (B_2H_6/SiH_4) remaining constant of 1.0%. The thin films with layer thickness of around 1 μm were deposited on about −1-mm-thick glass substrates at a temperature of 250 °C. The total pressure of reactive gases was 1.0 Torr. The detailed parameters of these samples are summarized in Table 1.

X-ray diffraction (XRD) and Raman scattering measurements performed at room temperature reveal that the B-doped nc-Si:H samples are nanocrystalline silicon with preferential growth orientation of (220) (see Fig. 1). The average grain sizes $d_{(220)}$ of the samples listed in Table 1 were obtained through the calculation from the full width at half maximum (FWHM) of the (220) diffraction peak by Scherrer formula. It is experimentally clear in Fig. 1(a) that the (220)-peak FWHM of sample A1 is slightly larger than that of sample A2, resulting in the smaller grain size of A1. Fig. 1(b) shows the two Raman spectra as measured from top surfaces of the thin films, with peak positions of 520.9 cm^{-1} for sample A1 and 524.3 cm^{-1} for sample A2. These Raman peak positions are blue shifted from that of crystalline Si (520.5 cm^{-1}), which is probably due to the combining effect of both compressive strain and phonon confinement within the B-doped nc-Si:H. The crystallinity X_c can be estimated from the Gaussian deconvolution of the Raman spectra. The experimental Raman spectra were fitted by four Gaussian phonon bands: amorphous longitudinal acoustic (LA) band with a

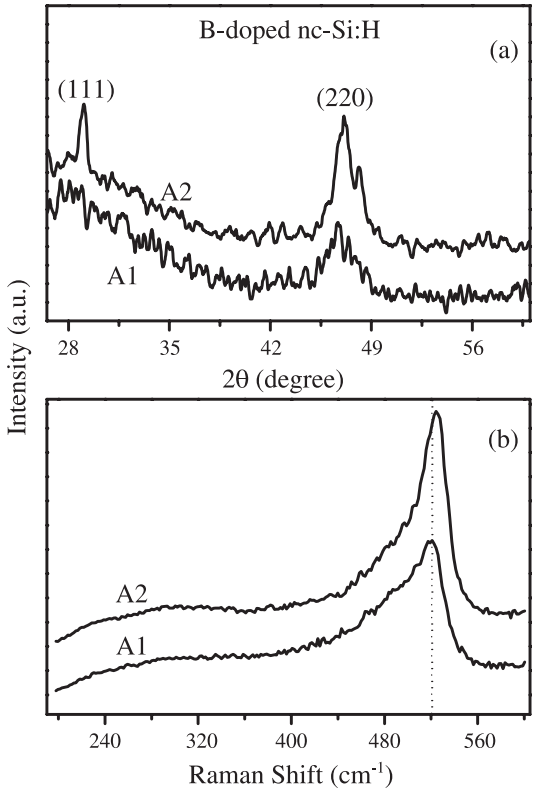

Fig. 1. (a) Experimental XRD results and (b) Raman spectra of the two typical B-doped nc-Si:H thin films deposited on glass substrates with different hydrogen dilution ratios.

Table 1
The parameters of the B-doped nc-Si:H thin films

Sample	H_2/SiH_4	$d_{(220)}$ (nm)	X_c (%)	A_{TL} (eV)	C_{TL} (eV)	E_{0TL} (eV)	E_{TL} (eV)	$\varepsilon_{1\infty}$	E_0 (eV)	E_d (eV)
A1	62.5	4.8	36	46.083	0.357	3.147	0.775	3.003	3.257	32.078
A2	97.1	5.1	47	54.889	0.410	3.312	0.996	2.751	3.412	31.687

$d_{(220)}$ is the average grain size obtained from XRD (220) peak, X_c is the crystallinity calculated from Raman spectra, A_{TL}, C_{TL}, E_{0TL}, E_{TL}, $\varepsilon_{1\infty}$ are the five parameters in the mTL model. Fits of the resulting refractive indices in the spectral range of 0.50–1.58 eV give the values of the two parameters E_0 and E_d within the WD model.

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