VIBRATIONAL AND ELECTRONIC PROPERTIES OF STRAINED α-Sn/Ge SUPERLATTICES

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(Received 4 August 1992)

Phonon spectra of strained α-Sn/Ge superlattices are studied using a generalized Keating model. General features of phonons are discussed. Effects of interface intermixing on Raman spectra are investigated by a supercell calculation. In addition, electronic band structures are calculated by a tight-binding method.

1. Introduction

Recently, the α-Sn/Ge system has received much interest because of its potential applications in novel devices, which might serve as alternatives to the Hg-Cd-Te system [1]. Semimetallic α-Sn is a zero-gap semiconductor, exhibiting a very high electron mobility owing to its small electron mass and the absence of polar phonon scattering. Therefore, the combination of zero-gap α-Sn and indirect-gap Ge may yield novel electronic band structures. In spite of the very large lattice mismatch of 14.7% between α-Sn and Ge, short-period strained α-Sn/Ge superlattices (SLs) have been successfully grown pseudomorphically on a Ge(001) substrate by a modified MBE technique [2].

2. Vibrational properties

In the present work, vibrational properties of α-Sn/Ge SLs are discussed by a generalized Keating model [3-5] which accounts for the strain effects properly. Values of Keating parameters for Ge are taken from Ref. 6 and for bulk α-Sn these parameters are determined by fitting to the experimental data.

2.1. General features of phonon spectra

Fig. 1 shows the calculated longitudinal and transverse phonon dispersion curves for an $(\alpha\text{-Sn})_2/(\text{Ge})_6$ SL grown on Ge(001) along the [001] direction. For longitudinal polarization (Fig. 1a), the top three modes are Ge-like confined LO modes with vibrations confined to the Ge layers. The mode around 230 cm^{-1} has finite dispersion with a significant acoustic-like excitation in Ge atoms. The mode below 220 cm^{-1} is a Sn-like quasi-confined LO mode since its frequency overlaps with the LA continuum of bulk Ge. Grown on a Ge(001) substrate, the Sn layers experience a tensile strain along the growth direction and an in-plane compressive strain. The frequency of the Sn-like mode is shifted upward considerably, which makes the frequency of the Sn-like quasi-confined LO mode (208 cm^{-1} at the zone center) slightly higher than that of the LO phonon at the zone center. The three modes in the low frequency range are the extended modes resulting from "folding" owing to the reduction in the Brillouin zone in SLs.

No interface modes are found in the longitudinal polarization because of the absence of gaps in the phonon spectra of Ge and α-Sn, similar to the observations in Si/Ge system [3-5].

For transverse polarization (Fig. 1b), there are two kinds of transverse modes, [110]- and $[1\bar{1}0]$-polarized, respectively. The top five modes are the Ge-like confined TO modes. The mode in the range of 160-180 cm^{-1}, is a true Sn-like confined TO mode since its frequency lies within the gap of the phonon spectra of bulk Ge. Between the Sn-like and Ge-like confined modes, two interface modes at 235 and 228 cm^{-1} appear. The frequencies of these modes lie within the gap of the phonon spectra of bulk Ge and α-Sn, so that neither Ge layers nor Sn layers can sustain the vibrations. These modes are sharply localized at the interface. No interface modes are expected in the [110]-polarization because the Sn-Ge bonds are all along the $[1\bar{1}0]$ direction.

It is found that the Ge-like LO modes can be well mapped onto the bulk dispersions by an effective wave vector $4\pi j/(n+1)a$, where j, n, and a are the order of a confined mode, number of Ge layers, and lattice constant, respectively. This relation is identical with that for Si-like confined LO modes found in Si/Ge SLs [4].

For Sn-like modes, the confinement is very

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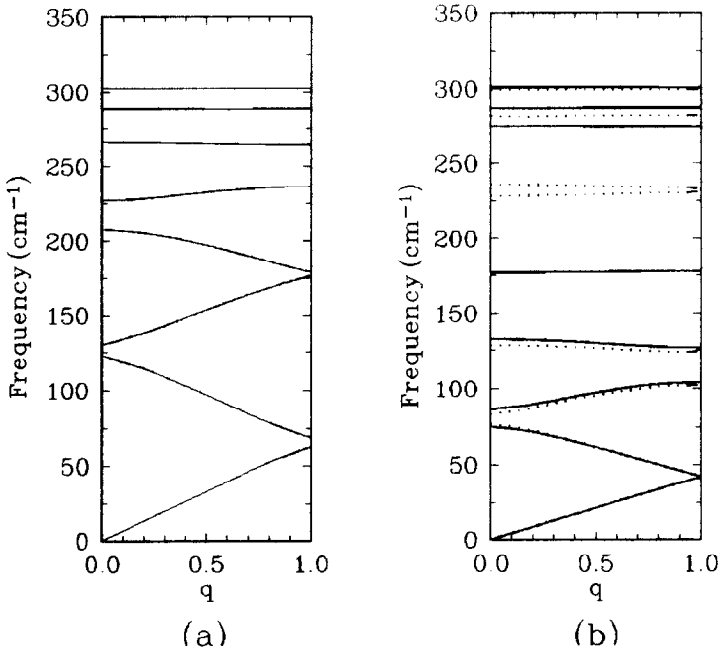

Fig.1 Calculated phonon dispersion curves along the [001] direction for an $(\alpha\text{-Sn})_2/(Ge)_6$ SL grown on Ge(001). (a) longitudinal modes; (b) transverse modes with solid and dot lines representing [110]- and [1$\bar{1}$0]-polarization, respectively.

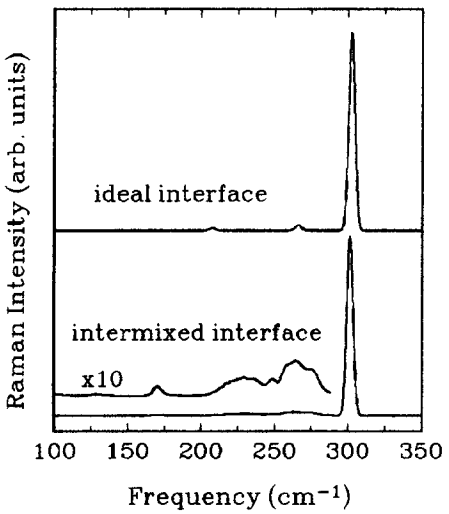

Fig.2 Calculated Raman spectra of an $(\alpha\text{-Sn})_2/(Ge)_6$ SL grown on Ge(001) with ideal (top) and intermixed (bottom) interfaces.

complex since their frequencies overlap with the LA continuum of bulk Ge. Strong LA-like excitations in Ge layers are expected.

2.2. Effects of interface intermixing

To discuss effects of interface intermixing, a supercell technique is used. In the supercell, the two-dimensional unit cell contains 8 atoms. The Ge and Sn layers nearest to the interface are allowed to exchange randomly to obtain the desired intermixing. Raman spectra are obtained by averaging over five distinct random configurations. Fig. 2 gives Raman spectra of an $(\alpha\text{-Sn})_2/(Ge)_6$ SL with ideal interface and with 38% exchange of interface Ge and Sn atoms. Obviously, Raman spectra are considerably modified by intermixing: the frequency of Sn-like LO mode are greatly shifted downwards and a new peak around 230 cm^{-1} appears. The peak around 230 cm^{-1} is caused by the introduction of interface intermixing, like the 400 cm^{-1} peak in Si/Ge SLs [4].

3. Electronic structures

The band structure of $(\alpha\text{-Sn})_m/(Ge)_n$ SLs are calculated by an empirical tight-binding method [7]. The second-nearest-neighbor parameters and spin-orbital splitting are taken into account. Fig. 3 shows the energy band near the gap for an

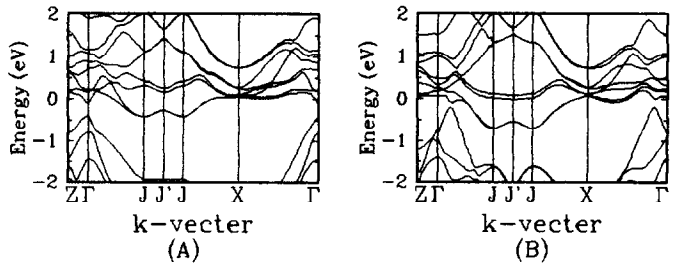

Fig.3 Band structure of $(\alpha\text{-Sn})_2/(Ge)_6$ SLs grown on (a) Ge substrate, (b) Sn substrate.

$(\alpha\text{-Sn})_2/(Ge)_6$ SL grown on Ge(001) and Sn(001) substrates. It is found that for Ge layers up to 6, the band gap are still zero, indicating that the SLs are semimetallic. This is more obvious for Sn substrate. While for a Ge substrate the difference between VBM at Γ-point and the CBM at J-point is only about 0.01 eV, indicating a change to semiconductor. In fact, the CBM relative to VBM for an $(\alpha\text{-Sn})_4/(Ge)_4$ SL is much lower than that for an $(\alpha\text{-Sn})_2/(Ge)_6$ SL grown on the same substrate, which indicates that metallicity increases with increasing Sn layers. A notable change in case of Sn substrate is that the VBM does not locate at the Γ-point. This is owing to the strong coupling between conduction band and valence band, which is an evidence of metallicity.

1. C.H.L.Goodman, IEEE Proc. **129**, 189(1982).
2. W.Wegscheider, K.Eberl, U.Menczigar, and G.Abstreiter, Appl. Phys. Lett. **57**, 875(1990).
3. Zi Jian, Zhang Kaiming, and Xie Xide, Phys. Rev. **B41**, 12862(1990);
4. J.Zi, K.Zhang, and X.Xie, J. Phys.: Condens. Matter **3**, 6239(1991).
5. J.Zi, K.Zhang, and X.Xie, Phys. Rev. **B45**, 8397 (1992).
6. R.M.Martin, Phys. Rev. **B1**, 4005(1970).
7. D.V. Jenkins and J.D. Dow, Phys. Rev. **B36**, 7994(1987).