Bandgap variation study of Si/Ge multilayers using Synchrotron radiation

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1. Introduction

In case of Si/Ge multilayers (MLS), differences in band gaps of elemental layers lead to discontinuities in valence band (VB) and conduction band (CB). Thus the electronic band structure may be tuned in these heterostructures by varying the individual layer thicknesses in the nanometer length scale and this fundamental concept may be regarded as bandgap engineering **[1]**. Considering the possibility of creating a variable bandgap material by controlling the micro-structural parameters of the MLS, the aim of the present study is to investigate the electronic properties and to determine the bandgap with annealing from the observed VB offsets using photoemission spectroscopy technique (PES).

2. Experimental

The [Si (5 nm)/Ge (5 nm)]$_{x10}$ MLS have been prepared by e-beam evaporation technique under UHV conditions at the deposition rate of 0.1 Å/s controlled using quartz crystal thickness monitor **[2].** PES measurements were carried out on the toroidal grating monochromator (TGM) beamline, Indus-1 **[3]** using pass energy of 30 eV. Samples were sputtered with low Ar^+ ions (~1 KeV and 1-2 μA) to remove the surface contamination as well as to reach the interface region in Si/Ge MLS. Micro-Raman measurements were performed on an integrated Raman system [Horiba Jobin Yvon HR800]. The excitation wavelength from HeNe laser was 632.2nm with a power of 9mW.

3. Results

3.1 PES measurements:

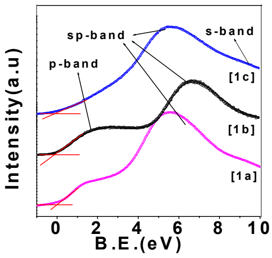

Fig.1: VB offset of Si/Ge

In our earlier published study, we have discussed the determination of bandgap of Si/Ge MLS using PES. For this, the required VB offsets were measured using the linear fit method **[4]**. The relation used was: $E_{gf} = \frac{3\Delta VB}{2} + E_{gb}$ where, E_{gf} is the bandgap of thin film (or MLS), ΔVB is the shift in the VB edge (VB offset) of the sample and E_{gb} is the bandgap of bulk material. Present study further extends this procedure and corresponding bandgaps are calculated with annealing. From earlier report, we have taken the value of bandgap of as deposited MLS. Taking the VB maximum of this sample as a reference point, we have determined the VB offset of annealed samples. Using the above-mentioned formula, the bandgaps were determined. Here we present the results for as-deposited and intermediate temperatures of 200°C and 400°C. The bandgaps show a systematically decreasing behaviour (as-deposited=1.83eV, 200°C=1.71eV, 400°C=1.62eV) [Fig. 1a, 1b and 1c respectively].

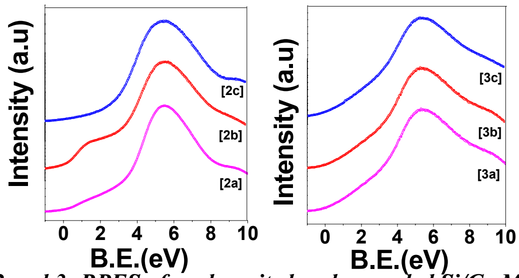

Fig.2 and 3: RPES of as-deposited and annealed Si/Ge MLS

These changes in the VB are reflected by the RPES measurements. Here we present a few of the spectra. For better comparison, all VB edges are shown without considering the offset. The p-band of the VB in as-deposited MLS is seen and enhances with energy variation from 70eV-134eV [Fig. 2a and 2b] and again reduces at 180eV [Fig. 2c]. Similarly, the s-band around ~9ev is also seen. Upon annealing, the p-band almost disappears [Fig. 3a] and also the sp- and s-bands are broadened. Here, no change occurs with variation in the photon energy.

3.2 Raman measurements

Figure 4 shows the Raman spectra of these samples at different annealing temperatures [as-deposited,200°C and 400°C]. It is clearly seen from the peak positions that the samples are nanocrystalline/amorphous having small grains as revealed from the shift towards lower wave number compared to corresponding bulks. Also, in as-deposited condition, very small amount of intermixed SiGe region is seen, which increases in intensity along with shift towards higher position upon annealing. This interdiffusion also leads to crystalline nature. The shift in Ge peak (265.9-286.05 cm^{-1}) is larger than Si (460.9-474.8 cm^{-1}). This can be attributed to lower crystallization temperature of Ge as compared to Si.

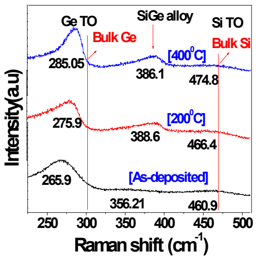

Fig.4: Raman of Si/Ge MLS

5. Discussion

In order to understand the decreasing behaviour of bandgap, it is necessary to take into account some factors like (i) roughness and interdiffusion at interface leading to the formation of SiGe alloy (ii) particle size etc. In the earlier publication, these effects were discussed in detail and the interdiffusion was found to be the strongest reason. Upon annealing, as observed from Raman, interdiffusion increases in intensity and is maximum for 400°C. This changes the environment of elemental atoms and thus the amount of VB offset changes. These changes are also reflected in RPES data, where drastic changes occur in the p-band structure of the VB. These changes contribute to the variation in the bandgap.

4. Conclusion

The VBPES has been employed to determine the bandgap of as-deposited and annealed Si/Ge MLS The variation in bandgap values is discussed in terms of the effect of various factors such as: (i) change in the intermixing leading to the formation of SiGe alloy upon annealing and (ii) roughness at the interface. The present experiments thus suggest the possibility of tailoring the bandgap of a material by changing the microstructural parameters of MLS in a controlled manner.

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