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Characterization of GeSi/Si Layer Structure by CBED

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Recently, there have been growing interests in GeSi/Si heteroepitaxial layers because of their promising optical and electronic properties which can be controlled through changing the composition of the epitaxial layer and hence strain field and defects distribution at the GeSi/Si interface. This work concerns strain field characterization through accurate measurement of lattice parameters across a GeSi/Si interface by CBED. In fact, the accuracy of lattice parameter measurement by CBED lies in that the angular resolution of a HOLZ/ZOLZ line is in reverse proportion to the amplitude of the relevant G vector. The larger the G vector, the higher the angular resolution is, and the easier the HOLZ line can be blurred by strain and defects. Therefore, there should be a compromise in between choosing the possibly largest G vector and the most distinct contrast of the HOLZ/ZOLZ lines concerned. In this work, nG_0 ZOLZ lines in off-axis double beam CBED patterns were employed in lattice parameter measurement when HOLZ line cannot be distinguished. Here G_0 is a ZOLZ reciprocal vector and n is an integer larger than 2.The GeSi/Si layered structure was prepared by growing GeSi layer on Si substrate with CVD.

Figure 1a is the XTEM image of the layered structure. A band of densely populated interface dislocations at the GeSi side indicates that the interface is relaxed. CBED [2 3 3] patterns taken at various points across the interface indicate that as long as the probe is placed outside the dislocation band, the position of the electron probe will have no evident effect on HOLZ line distribution and spatial resolution of HOLZ lines, meaning that there is no strain outside the dislocation band (CBEDP's taken from points 1,2 and 3 are shown in figures 1b,1c and 1d). However, the CBED pattern taken from inside the dislocation populated band (Figure 1c) is severely distorted, in which HOLZ lines cannot be distinguished. Therefore, strain was not completely relaxed within the dislocation band. The acceleration voltage was calibrated as 201 KV and the lattice parameter for GeSi is then determined to be 5.4685 Å through HOLZ line simulation. The Ge concentration can then be determined as 17at% according to the change of lattice parameter[J P DISMUKES, et al: J. Phys. Chem. **68**, 1964, p3021]. The off-axis CBIM taken from the interface(Figure 1e) shows the displacement of ZOLZ lines at the interface, revealing the orientation difference between GeSi and Si due to relaxation. It is important to note that the off-axis CBED pattern taken from the same spot as Figure 1c can reveal clearly the (8 8 0) ZOLZ line with good spatial resolution. The (2 2 0) d-spacing for points 1, 2 and 3 has been determined according to the spacings of the relevant (8 8 0) ZOLZ line pairs as 1.9194 Å, 1.9282 Å and 1.9350 Å respectively. It is worth noting that the lattice spacing at point 3 is very close to the result from normal CBED pattern (figure 1d, 1.9337 Å). According to the change in lattice spacing, the relaxation at GeSi/Si interface can be deduced as 62% .

The conclusion of the present work is that CBED is an accurate method for determination of lattice parameters and as long as the relationship between composition and lattice parameters is available, it is also an accurate method to determine alloy composition. With the assistance of off-axis CBEDPs, CBED has good feasibility for the characterization of strained layer structures. The authors wish to thank Dr F. Namavar for the provision of samples. Two of the authors (GS and ZY) are grateful to Chinese government and British Council for financial support through FBFSS.

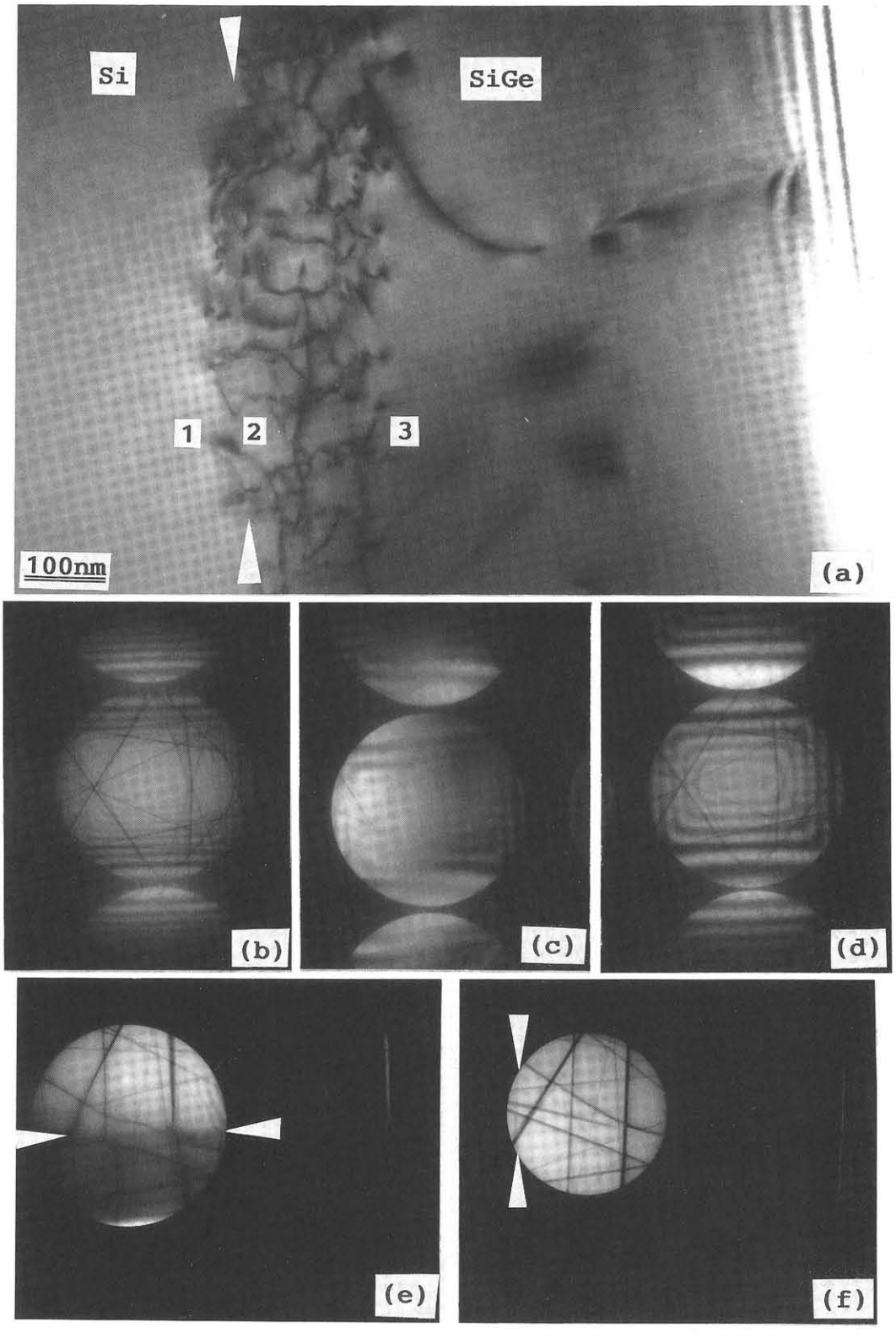

Figure 1: Cross sectional TEM (XTEM) image of a GeSi/Si layered structure(a) with an arrow indicates the interface, CBEDPs(b, c, d, f) and an off axis CBIM with interface indicated (e).