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Title: DEFECT STRUCTURES IN SEMICONDUCTING RHENIUM DISILICIDE EPITAXIAL THIN FILMS

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DEFECT STRUCTURES IN SEMICONDUCTING $ReSi_{2-x}$ EPITAXIAL THIN FILMS

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Narrow band gap semiconductors such as $ReSi_{2-x}$ (Eg ~ 0.12 eV) are potential materials for infrared detectors [1]. Further, $ReSi_{2-x}$ is in thermodynamic equilibrium and has a very small lattice mismatch with Si offering the potential of developing $ReSi_{2-x}$/Si heterojunction devices where the detector element and the signal processing circuitry can be integrated on one Si chip. In a previous study, strong crystallographic alignment between $ReSi_{2-x}$ film and (001)Si substrate was observed by ion channeling [1]. In this study, a transmission electron microscopy (TEM) study has been performed on $ReSi_{2-x}$ epitaxial films on (001) Si. Comparisons are made to our previous microscopy study [2] on the defect structures in bulk single crystals of $ReSi_{2-x}$.

$ReSi_{2-x}$ films were prepared by reactive deposition epitaxy (RDE) technique by evaporating Re onto (001) Si wafer at 650 °C. A cap layer of Cr was evaporated at room temperature. A bright field (BF) TEM image of the interface in cross-section is shown in Fig. 1 with the corresponding selected area diffraction pattern (SADP) shown in Fig. 2. Voids are observed along the interface, though the majority of the interface area was found to be clean of voids or oxide and hence, epitaxial growth of the film was possible. Such voids have been observed in other RDE growth as well, e.g. SiC on Si [3]. Presumably, in the early stages of growth, islands of silicide form on Si substrate and for subsequent growth Si is continuously extracted from the substrate by preferential outward diffusion along the side surfaces of the silicide islands causing voids to form. The orientation relationship was (001)Si // (010)silicide, [110]Si // [001]silicide and the SADP in Fig. 2 shows two variants of this relationship with [110]Si, [001]silicide and [100] silicide zone axes patterns superimposed. Silicide spots are indexed according to the body-centered tetragonal (bct) $MoSi_2$ structure. Weak orthorhombic (~0.5%) and monoclinc distortions from the bct structure observed in bulk $ReSi_{2-x}$ were not discerned in the diffraction patterns from the thin films. Good epitaxy is expected since the face diagonal of Si ($a\sqrt{2}$) is equal to the c lattice parameter of silicide. The silicide layer shows planar defects on the c planes and corresponding streaking in the silicide diffraction spots. In order to study these defects in detail, high resolution TEM was performed and a HREM image, for the same orientation as in Fig. 1 but from a region with no interfacial voids, is shown in Fig. 3. The planar defects are very closely spaced and since two variants ([001] and [100] orientation of silicide) are present both parallel to the cross-section shown and in the thickness direction of the TEM foil, clear images showing the atomic structure of the silicide are not observed. Some unit cells corresponding to the [100] and [001] orientations of the $MoSi_2$ structure are highlighted by rectangular and square boxes respectively in Fig. 3. The HREM images from these "good" regions could be simulated using MacTempas assuming the $MoSi_2$ structure. For the $ReSi_{2-x}$ film to be a semiconductor, the unit cell must have an even number of valence electrons and this is possible with a stoichiometry of Re_4Si_7 and not with $ReSi_2$. Two unit cells of the $MoSi_2$ structure (4 Mo atoms + 8 Si atoms) viewed along [100] are shown in Fig. 4(a). The removal of one (001) Si layer every two unit cells (Fig. 4(b)) would give the stoichiometry of Re_4Si_7. The high density of planar defects observed on (001) may correspond to collapse and shear of the missing Si layers. This defect structure is different from that observed in bulk single crystals that exhibited the Nowotny "chimney-ladder" structure where the Si sub-lattice parameter was different from the Re sub-lattice parameter and the resulting structures were either incommensurate (Si sub-lattice parameter was not an integer multiple of Re sub-lattice parameter) or commensurate (Si sub-lattice parameter was an integer multiple of Re sub-lattice parameter). Further studies on the effects of annealing and alloying with Mo on the defect structure of Re_4Si_7 films is in progress.

References

1. J.E. Mahan, G. Bai, M.-A. Nicolet, R.G. Long and K.M. Geib, Thin Solid Films, **207**, p223 (1992).
2. A. Misra, F. Chu and T.E. Mitchell, Phil. Mag. A, **79**, (1999), in press.
3. L.-O. Bjorketun, L. Hultman, I.P. Ivanov, Q. Wahab and J.-E. Sundgren, J. Cryst. Growth, **182**, p379 (1997).

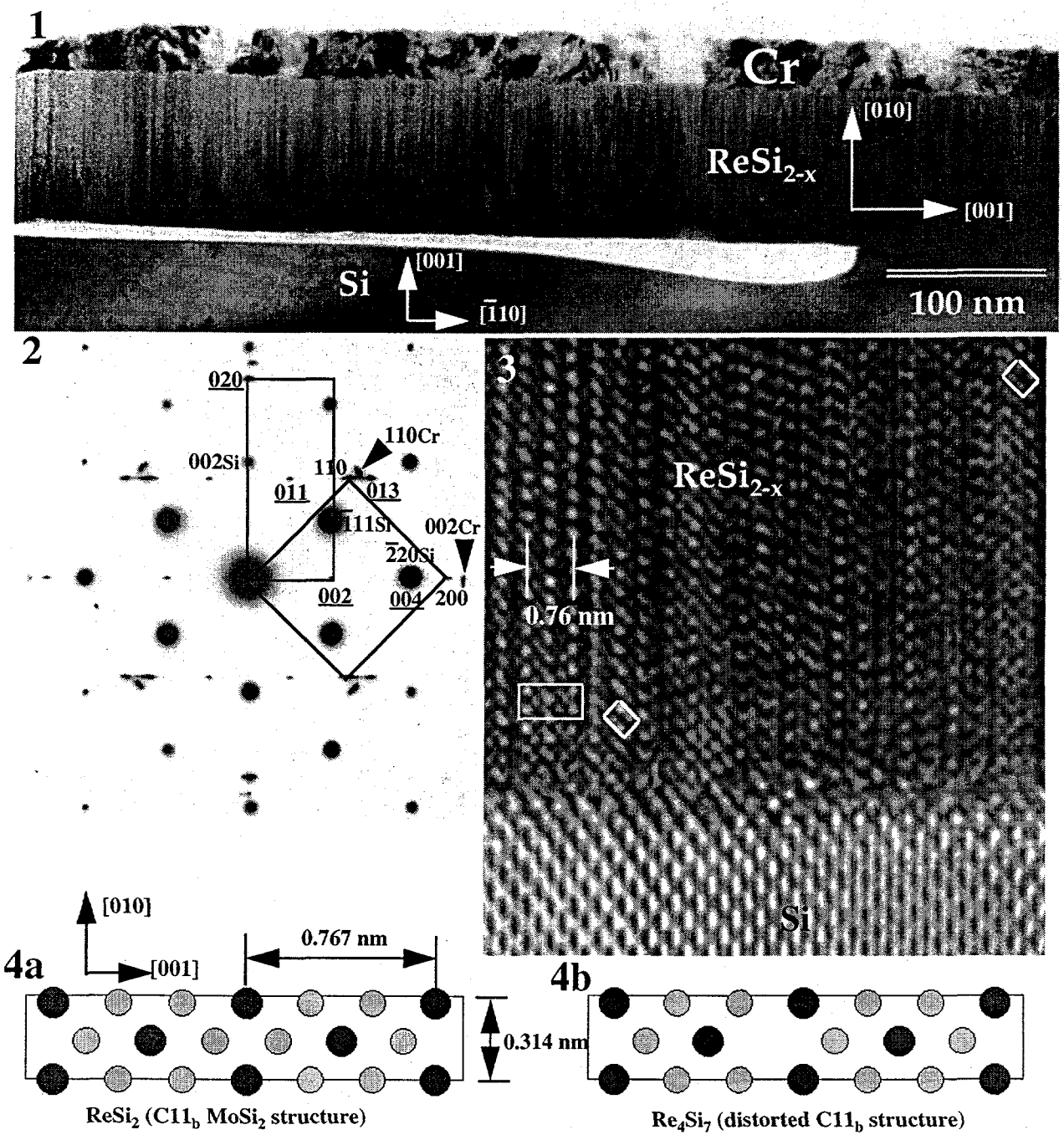

Fig. 1 BF TEM image showing the $ReSi_{2-x}$/Si interface in cross-section. Note the interfacial voids and planar defects on (001) in the silicide.

Fig. 2 [110]Si //[100]silicide//[001] silicide zone axes SADP corresponding to Fig. 1. The [100] silicide pattern is shown by a rectangular box and spots underlined. The [001] silicide pattern is shown by a square box. Spots from Si and Cr are labelled.

Fig. 3 HREM image of the $ReSi_{2-x}$/Si interface (same orientation as Fig. 1) in cross-section from a region with no interfacial voids.

Fig. 4 Schematic illustration, projected along [100], of (a) 2 unit cells of $ReSi_2$ with bct $MoSi_2$ structure, and (b) same with one (001) Si plane missing every 2 unit cells to give Re_4Si_7.