11-Surfaces, Interfaces and Thin Films

PS–11.01.08 DIRECT IMAGING OF O-LATTICE OF INTERFACES IN Ti(CN)-TiB_2-Ni CERAMICS. By J.Y. Dai, D.X. Li and H.Q. Ye, Laboratory of Atomic Imaging of Solids, Institute of Metal Research, Academia Sinica, Shenyang 110015, China.

The mixture with the compositions of 57.6 wt% TiB_2, 40.4 wt% Ti(CN) and 2 wt% Ni was hot pressed in vacuum at 1850 °C and 25 MPa. During the sintering process, precipitation of second phase and segregation of impurities have occurred. The average grain size of the ceramics is about 1 μm. Two kinds of orientation relationships (O.R.) between FCC Ti(CN) and hexagonal TiB_2 were detected by means of electron diffraction and high resolution electron microcopy, i.e. O.R. I: $[\bar{1}10]_{Ti(CN)}//[2\bar{1}\bar{1}0]_{TiB2}$, $(111)_{Ti(CN)}//(0001)_{TiB2}$ and O.R. II: $[\bar{1}10]_{Ti(CN)}//[2\bar{1}\bar{1}0]_{TiB2}$, $(001)_{Ti(CN)}//(01\bar{1}0)_{TiB2}$. In general, Ti(CN) and TiB_2 phases oriented at random. When these phases grew together immediately, they coexist with a unique orientation relationship of O.R. I. Ti(CN) particles with a size of a few nm were also precipitated in TiB_2 crystals. Fig.1 shows the typical morphology of TiB_2-Ti(CN)-Ni ceramics with TiB_2 and Ti(CN) grew together and Ti(CN) particals precipitated in TiB_2 crystals. Besides O.R. I, a different orientation relationship called O.R. II between Ti(CN) precipitates and TiB_2 can be detected occasionally.

O-lattice calculations between FCC Ti(CN) and hexagonal TiB_2 interfaces were carried out for those two orientation relationships. For O.R. I, the calculated O-lattice unit cell is hexagonal and the primary dislocation networks is also hexagonal by duality relations. However, no primary dislocation was found in the HREM image. The small mismatch (about 1%) has been accommodated by elastic strain and/or secondary dislocation networks, and the calculation of secondary O-lattice agree well with the observed secondary dislocation networks. Ti(CN) precipitates were hexagonal in shape and the ledges or facets are parallel to edges of precipitation. These can be interpreted by O-lattice theory.

For O.R. II, the calculated O-lattice unit cell is tetragonal body, and the Ti(CN) precipitate also shows a tetragonal body in shape. HREM image of Ti(CN)/TiB_2 interface shows that there are many steps with the height equal to one layer of atomic plane and average interval of seven $(0001)_{TiB2}$ interplanar spacing. O-lattice theory analysis points out that this step structure is the optimal low energy interface which passes through coherent region as many as possible.

In prensent case, intergranular phases were also detected at grain boundaries, which indicated by small black dots with white circular delineation in Fig.1. Two Ni-rich intergranular phases which containing Ti and Si, Fe impurities were found to be $Ni_{31}Si_{12}$ and $Ni_{16}Ti_6Si_7$ type structure.

PS–11.01.09 DETERMINATION OF STRAINS IN $Hg_{1-x}Cd_xTe$ THIN FILM MATERIAL. By Fuju Yu* and An Yang, Shanghai Institute of Technical Physics, Academia Sinica, Shanghai, China

$Hg_{1-x}Cd_xTe$ epitaxial layers grown by MBE, LPE are among the most important semiconductor materials widely used for making infrared focal plane devices.However those films are generally composed of highly lattice-mismatch layers and mutational composition areas due to properties of type 2-6 compounds, and lattice strain and composition mutation can sometimes not been accommodated by buffer layer and further interfere seriously epilayers.The study of lattice mismatch strain (Basson, et al. 1983) , composition mutation, and intensive strain field which created from substrate and acrossed all epilayers was nondestructively carried out by X-ray double crystal diffraction and X-ray topography.

It is useful that FWHM (half width of rocking curve from double crystal diffraction) value as a criterion of structure quality for epitaxial $Hg_{1-x}Cd_xTe$ films. FWHM at 153 arcsec. was measured for MCT1037 wafer including three layers grown by MBE on GaAs substrate, (N,-N) set, $CuK\alpha_1(422)$ reflection. This is a better result but still much large than theoretic one (less than 40 arcsec.), it attributes to lattice mismatch at the bounderies of heterolayers. Double crystal diffraction with high resolution is taken for measuring lattice mismatch in hetrojunction (Cohen, 1967). Measuring a heterojunction $Hg_{1-x}Cd_xTe$/CdTe LE92-5 grown by LPE on CdTe(111) substrate, two diffraction peaks appear on the rocking curve due to different lattice parameters of epilayer and substrate. The lattice mismatch at 0.27% is obtained from the difference of angles corresponding with the two peaks, then composition calculation in epilayer is carried out from Vagar's law, composition x=0.14 much approaches to the expected one. An unhomogeneously growing of $Hg_{1-x}Cd_xTe$ film on MBE was also studied by a gradual transition layer of composition Δx revealed with double crystal diffraction.

X-ray topography is also available for checking the quality of $Hg_{1-x}Cd_xTe$ epilayers (Yu Fuju, 1990). A topographic pattern of a wafer MCT410 shows that the intensive strain field on substrate propagates through the buffer layer, the layer with expected composition, the dull layer and so on, while the thin films are grown by MBE. From this point, it is very important to improve the polishing technology of substrate.

References

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PS–11.01.10 ADSORPTION OF HYDROGEN, OXYGEN AND SULFUR ON Cu(110) STUDIED BY LEED. By R. Zuschke, T. Grünberg, J. Wever, S. Pflanz, M. Burghammer, D. Baraitaru, D. Wolf and W. Moritz, Institut für Kristallographie und Mineralogie, Universität München, Fed. rep. of Germany

The different adsorbate structures and adsorbate induced reconstructions on the Cu(110) surface have been studied by LEED I/V and beam profile analysis. Hydrogen causes a (1x2) reconstruction of the missing row type, the hydrogen coverage is 0.5 monolayers (ML). It is adsorbed either in two-fold or four-fold

