

**07.2-12 MEASUREMENT OF NONUNIFORM ELASTIC STRAINS IN EPITAXIAL THIN FILMS.** By W. E. Mayo, J. Chaudhuri and S. Weissmann, Department of Mechanics and Materials Science, College of Engineering, Rutgers University, Piscataway, N.J. 08854, USA.

A new X-ray method is presented for determining elastic strains with high precision in single crystal materials. This method is significant not only in its ability to determine the full elastic strain tensor but also its distribution about a strain center with a resolution of approximately 60  $\mu\text{m}$ . This method employs the recently developed Computer Aided Rocking Curve Analyzer (CARCA) (Yazici, Mayo, Takemoto and Weissmann, *J. Appl. Cryst.* (1983) 16, 89) and is particularly well suited for analysis of thin film structures common to electronic materials. In the present method, the elastic strain analysis of Imura et al. (Imura, Weissmann and Slade, *Acta Cryst.* (1962) 15, 786) is carried out on a point by point basis for up to 12 reflections, thus yielding the local strain at each corresponding point on the sample. In this paper the operating principle of the method will be described and potential applications will be presented. Among these are the generation of long range strain concentrations at dielectric steps, epitaxial interfaces and diffused metal contacts. Also, for epitaxial structures, it is possible to utilize the method to measure the uniformity of the film thickness. As an example of the power and sensitivity of the method, a study of the strain distribution in an InGaAsP epitaxial film on an InP substrate will be presented.

#### KEY WORDS

Elastic Strain Determination  
Non Uniform Strain Distribution  
Epitaxial Films

**07.2-13 COMPUTED AND REAL TRANSMISSION ELECTRON MICROSCOPE IMAGE CONTRASTS FROM GRAIN BOUNDARIES.** By M.J. Turunen and H.O. Martikainen, Laboratory of Physical Metallurgy, Helsinki University of Technology, SF-02150 Espoo 15, Finland.

The resolution attainable in a modern transmission electron microscope is good enough to resolve a number of fine structural features in grain boundaries of metals. Commonly observed periodic contrast images are interpreted in terms of grain boundary dislocations. The analysis of lattice dislocations is principally based on the invisibility criterion,  $g \cdot b = 0$ , where  $b$  is the Burger's vector, chosen from the known possibilities of lattice displacements, and  $g$  is the diffraction vector. This method does not readily yield itself to the interpretation of grain boundary dislocation images, since there is much wider choice of possible Burger's vectors, and the value of  $g \cdot b$  may be quite small in any case. Also the dislocations are often so close together that the validity of the invisibility criterion is doubtful. Therefore, more sophisticated techniques are needed, such as the image matching method, in which a computer calculated image is compared with the observed one.

In this contribution we present a practical computer calculation method for contrast images and a number of examples, in which the calculated images are compared with real ones. Our approach differs somewhat from the one presented by Humble and Forwood (P. Humble and C.T. Forwood, *Phil. Mag.* (1975) 31, 1011). Applying our calculation technique it is possible to include an arbitrary number of dislocations and

their elastic fields, also the type of the dislocations can be arbitrary as well as their density and arrangement. A limitation in our method is that we can use only isotropic elasticity.

It is assumed that the lattice displacement near the grain boundary affecting the contrast arises only from the dislocations. The displacement is calculated by summing up the contributions from each individual dislocation segment. The contribution of one segment is obtained by using formulae derived from the Burger's equation (cf. J.P. Hirth and J. Lothe, *Theory of Dislocations* (1982) p. 101). The Howle-Whelan equations for the two beam case are solved by using the matrix method as proposed by Thölen (A.R. Thölen, *Phil. Mag.* (1970) 22, 175). The constructed computer program calculates the direct and diffracted intensity in 96x56 separate columns through the specimen, which consists of two crystals separated by the boundary plane. The relative orientation of the crystals can be arbitrary, and either one or both of them can be oriented for two beam diffraction. In the case of one of the crystals not being oriented for two beam diffraction only absorption effects are considered in the part of a column that belongs to that crystal.

As an output device for the computed images we have used numerically controlled graphical scanner, which plots the pictures on a photographic film. In this way their quality is comparable to actual pictures taken with an electron microscope.

**07.2-14 X-RAY DIFFRACTION DETERMINATION OF STRESSES, TEXTURE, CRYSTALLITE SIZE, MICROSTRAIN AND COMPOSITION IN WEAR-RESISTANT TITANIUM CARBIDE LAYERS.** By W.G. Sloof, R. Delhez, Th.H. de Keijser and S. Radelaar, Delft University of Technology, Laboratory of Metallurgy, Rotterdamseweg 137, 2628 AL Delft, The Netherlands.

Thin titaniumcarbide ( $\text{TiC}_x$ ) layers were Chemically Vapour Deposited (CVD), with and without a carbon source ( $\text{CH}_4$ ) in the gas phase on iron substrates with 0.06-1.20 wt.% C. The strength of the 110 fiber texture present depends on the wt.% C and on the presence of  $\text{CH}_4$ . A biaxial state of compressive stress exists with the two principal stresses equal. The substrates show a tensile stress. The observed stresses are quantitatively explained from the difference in thermal shrinkage (including phase transformations) between layer and substrate during cooling from the deposition temperature to room temperature. The carbon content  $x$  of the  $\text{TiC}_x$  layers was determined from the strainfree lattice parameter obtained from the data of the  $\sin^2\psi$  method. The carbon content is:  
- practically independent of the carbon content of the substrate for substrates with more than about 0.3 wt.% C,  
- highest near the substrate and its gradient is almost zero near the free surface and  
- significantly larger for layers deposited with  $\text{CH}_4$  than for layers deposited without  $\text{CH}_4$  in the gasphase. The crystallite size of the layers on the substrates with more than 0.3 wt.% C is almost independent of the carbon content of the substrate. This applies to layers deposited with and without  $\text{CH}_4$ . The microstrain however increases with the carbon content of the substrate. The microstrain of layers deposited without  $\text{CH}_4$  is larger than of layers deposited with  $\text{CH}_4$ . Lattice imperfections and/or fluctuations in the composition of TiC appear to be the main contributions to the microstrain.