Figures 3 and 4 demonstrate the use of the modified method for dislocation B in Figs. 1-2. It is shown that only two images (for example , 1a and 2c) are sufficient to determine the parity and the Burgers vector of the dislocation. Indeed, figure 1a represents the weak image of dislocation B which corresponds to a vanishing contrast owing to $\mathbf{g_0 b}=0$. The residual contrast is the result of $\mathbf{g_0 b\times l}=0$. Using the oscillations or image shift on fig.2c one can determine the parity P=1 as well as the direction of the the projection **e'** of the **e**-vector on the image plane by analysing the halo contrast (table 1). As **(111)** and a/2<**110**> are the favourable types of glide plane and Burgers vector respectively in the zinc-blende structure one can propose four orientations possible for **e** $(\mathbf{111}, \mathbf{\bar{1}11}, \mathbf{1\bar{1}1}, \mathbf{\bar{1}\bar{1}1})$ and **b** $(\mathbf{011}, \mathbf{0\bar{1}\bar{1}}, \mathbf{0\bar{1}1}, \mathbf{01\bar{1}})$ in accordance with the stereographic (001) projection for a cubic crystal (figure 4). Based on the information on the dislocation sign deduced above one can conclude that vector $\mathbf{e_B}=[\mathbf{\bar{1}\bar{1}1}]$ and, then, $\mathbf{b}$=a/2$[\mathbf{0\bar{1}\bar{1}}]$ if $\mathbf{l}=[\mathbf{\bar{1}32}]$ (see table 2). Dislocation A can be analysed analogously.

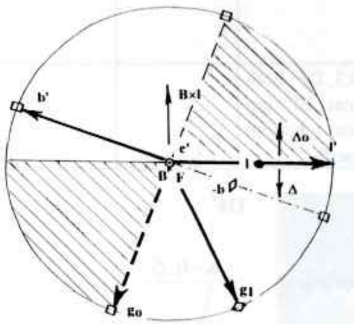

Figure 3. The determination of the parity P. **l'** is projection of the dislocation line **l** onto the image plane.

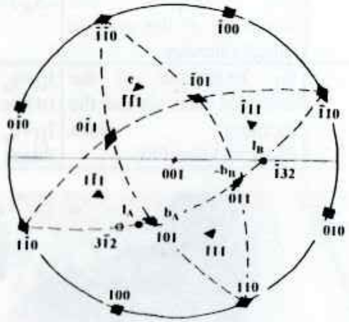

Figure 4. Stereographic (001) projection of a cubic crystal. The normal of foil **F** and beam vector **B** are close to the interface normal **n=[001]**.

The modified analysis of Burgers vectors can be applied, e.g., to dislocations in semiconductors where only parts of loops are visible so that the inside-outside technique fails. The investigation of a lot of dislocations such as, e.g., A and B in Fig.1 reveals that dislocations having the same glide planes are created in deformation centres at the interface under residual stresses during growth or postgrowth cooling. The nature of such deformation centres was discussed elsewhere (Yavich et al 1991) and can be associated with the small Al_2O_3 precipitates in AlGaAs epilayers. Dislocation loops gliding from the centre to the surface grown break into two segments which are almost parallel to the Burgers vector **b** . Therefore, most of the threading dislocations observed in epilayers have a large screw component of **b**. Dislocations A and B represent two segments of different dislocation loops created by the same deformation centre.

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Dislocation parity analysis applied to unify the Burgers vector determination by TEM

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ABSTRACT: Based on a refinement of the Marukawa's analysis of dislocation contrast features we propose a modified method of identifying the Burgers vector **b**. High voltage electron microscopy (HVEM) as well as computer simulation technique were applied to study the contrast behaviour of mixed dislocations with a large screw component of Burgers vector under different diffraction conditions and to check the validity of the method proposed. The analysis of the contrast oscillations and the image shift relative to the projection of the dislocation line enable us to determine the "dislocation parity" P=sign[**l×b.B**] while the halo contrast can be used to define the orientation of the "additional halfplane" or vector **e=l×b/|l×b|** in the image plane. The applicability of the method of determining dislocation parameters in heterostructures is demonstrated.

1. INTRODUCTION

In transmission electron microscopy (TEM) the Burgers vector of a dislocation is usually identified in at least by three different ways . The first one is based on the invisibility criterion **gb**=0 , where **g** is the diffraction vector and **b** is the Burgers vector (Hirsch et al 1965). In general, two noncomplanar **g** vectors fulfilling the invisibility criterion are necessary and sufficient to determine uniquely the **b**-axis. Difficulties arise if the invisibility rules cannot be strictly applied as, e.g., in cases of anisotropic media, for certain mixed or partial dislocations, for many beam excitations or if two noncomplanar vectors **g** can't be found owing to experimental limitations (Scheerschmidt 1987). In measuring the **b**-axis the most important restriction, however, is the impossibility of generally determining the direction of **b** by using the invisibility criterion. Thus it is necessary to gain further information by analysing contrast details (e.g. image shift, contrast oscillations, symmetry) or by applying inside-outside (Föll & Wilkens 1975) or halo (Rozhanskij et al 1981) contrast methods to define the **b** direction. Image simulation or the matching technique (Head et al 1973) is the second possibility. Being quite reliable without parameter determination directly from the experiment or by using the other methods discussed here this method has a degree of freedom far too large in the parameter space. The large degree of freedom can be reduced by the predominance of some of the parameters applying the invisibility rule or by analysing contrast details again. The third method, proposed by Marukawa (1979) makes use of characteristic image features such as their asymmetry related to the signs of **gb** and **g(b×l)** where **l** is the dislocation line vector. Analysing the image asymmetry at different reflections **g**, the probable orientation of the Burgers vector can be revealed to lie in so small a solid angle that it is possible to choose **b** directly from crystallographically allowable vectors. Being rather suitable in practice the method has some restrictions, too, for example, for dislocations lying parallel to the foil surface.
On the other hand, in most practical cases one **g** vector fulfilling the invisibility criterion can be found rather easily. Therefore, the combination of the methods mentioned above may be more convenient for investigating dislocations. Based on a refinement of Marukawa's analysis of contrast features the modified method can be proposed to determine the dislocation sign or dislocation parity in respect of the axis chosen.

2. DISLOCATION PARITY AND PARAMETERS OF CONTRAST FEATURES

The Burgers vector **b** of a dislocation is a pseudo-vector and fixed only in relation to the dislocation line vector **l** (FS/RH rule: Finish-Start/Right Hand). Nevertheless, the direction of **b**, also called sign of **b** or dislocation sign, is important for intrinsic/extrinsic types of defects, the position of the "extra half-plane" **e**=**l**×**b**/|**l**×**b**| and so on. Especially for heterostructures the sign of the dislocation is strongly connected with the misfit in the lattice parameters of the epilayer a_l and the substrate a_s. Indeed, the position of the additional halfplane related to the interface normal **n** depends on the misfit sign so that sign[**l**×**b**.**n**]<0 for $\Delta a=a_l-a_s>0$, and vice versa. The contrast characterizing parameters n=**gb**, p=**gb**$_e$, m=**g**(**b**×**l**)/8 (width, symmetry, visibility) and also such features as, e.g., halo contrast, image shift and black-white oscillations are thus determined by the dislocation sign. According to the unification of the analysis, the beam vector **B** turning to the electron gun (Head et al 1973), should be chosen as the basis of a fixed coordinate system. Defining the parity P=sign[**l**×**b**.**B**]=sign[**e**.**B**] and relating the parameters to the beam **B** as shown in table 1 by extension with [**l**×**B**] a consistent and unique description can be gained.

3. EXPERIMENT AND SIMULATIONS

HVEM (1 MV) was applied to a 2μm (001) AlGaAs/GaAs heterostructure grown by liquid phase epitaxy to study the contrast behaviour of the threading dislocations under different diffraction conditions. For electron microscopy the specimen was first prepared by chemically removing the substrate using a polishing solution, and finally by ion milling down to thickness of about 0.45 μm. Image simulations were performed using the two-beam approximation of dynamical scattering in the Howie-Whelan formulation (see e.g. Scherschmidt 1987).

4. RESULTS AND DISCUSSION

Figures 1 and 2 represent electron microscope micrographs and corresponding simulated images of two mixed dislocations (A and B) with a large screw component of the Burgers vector under different diffraction conditions. For the parity analysis the oscillating contrast as well as the image shift can be used, whereas the halo contrast yields the information about vector **e**. A connection of the dislocation parity with the projections possible of the **b** vector can be clearly seen from the equation P=sign(**Be**)=sign(**B**.**l**×**b**)=sign(**B**×**l**.**b**) (see figure 3).

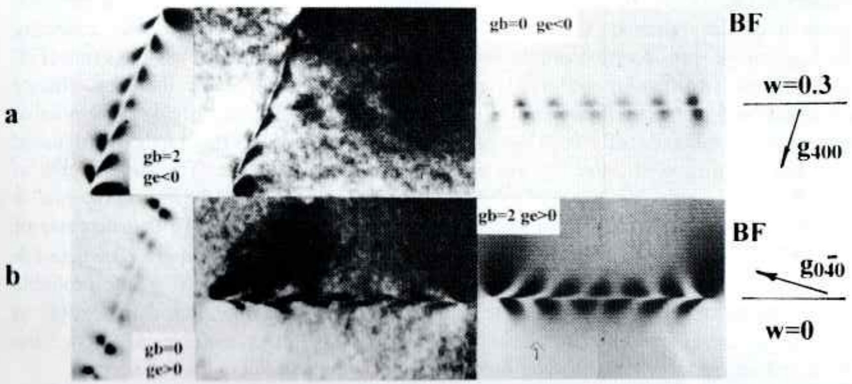

Figure 1, a-b. Experimental (central) and corresponding simulated images of the mixed dislocations A (left) and B (right) at the reflections of <400> type excited (|**gb**|=0 or 2).

Table 1. Contrast features of dislocation images in dependence on the dislocation parameters and diffraction conditions.

Contrast	Contrast parameter	Dependence	Validity region	Parity P	Restrictions
Contrast oscillations near the surface	Δ_0: black-white vector, drawn from the centre of the black spot to the centre of the dark one at the end of dislocation oscillation contrast	Δ_0=(**gb**)[**l**×**B**]	Inclined dislocation, **gb**≠0, BF: both ends, DF: top end, bottom - reversed	-sign($g_1\Delta_0$)	g_1 belongs to the one of two biggest (>90°) solid angles bounded by **l'** and g_0-axes
Image shift	Δ: shift vector drawn normal to the dislocation line towards the minimum of the average image intensity	$\Delta=-\Delta_0\, s\sqrt{1+1/w^2}$	**gb**≠0, w≠0	sign($g_1\Delta w$)	the same as above
Halo contrast	I_H: Brightness of the extended halo around the merging point dislocation-surface	$I_H>I_0$ if **ge**>0 (white halo) $I_H<I_0$ if **ge**<0 (black halo)	|w|≤0.3, DF: both surfaces, BF: top surface, (bottom reversed)		

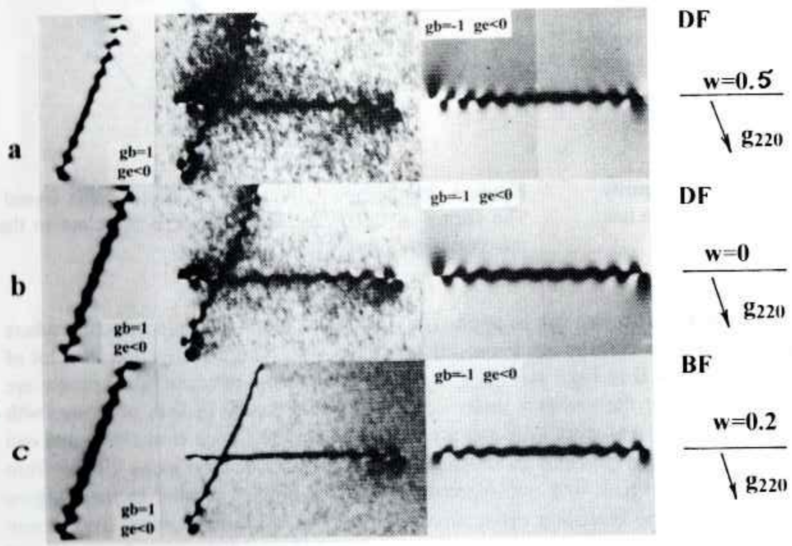

Figure 2. Images at reflection **g**=220 excited (|**gb**|=1) and different w values.

The algorithm of the modified method can be summarized as follows. At first, based on the invisibility criterion g_0**b**=0 for one g_0-vector the projection of the **b**-axis on the image plane should be determined (first image). Then, analysing the features listed in table 1 for a second image at g_1**b**≠0 one can define the dislocation parity P and **e**-vector (figure 3-4) and , thus, the dislocation sign related to the axes chosen will be determined. According to the object crystallography several axes probable for **b** vector can be concluded from this and, then, **b**-vector can be uniquely defined if **l'**-direction is chosen.

Table 2. The parameters of dislocations (A and B) under study and diffraction conditions.

Disloca-tion	l [hkl]	b [hkl]	e [hkl]	g_{400} n	(fig. 1a) sign(m)	$g_{0\bar{4}0}$ n	(fig1.b) sign(m)	g_{220} n	(fig.2) sign(m)	P
A	$3\bar{1}2$	a/2[101]	$\bar{1}\bar{1}1$	2	-1	0	+1	+1	-1	1
B	$\bar{1}32$	a/2[$0\bar{1}\bar{1}$]	$\bar{1}11$	0	-1	2	+1	-1	-1	1