11.7-3 STATIONARY WAVES FROM A SINGLE HETEROSTRUCTURE ON GaAs - A COMPUTER EXPERIMENT. By A. Authier[1], J.Gronkowski[2] and C.Malgrange[1]. [1]: Laboratoire de Minéralogie-Cristallographie, CNRS et Universités Paris VI et VII, France; [2]: Institute of Experimental Physics, University of Warsaw, Poland

Two of the most promising applications of the Stationary Waves method for the localization of atomic positions are the study of solid-solid interfaces and that of implanted layers. In both cases, the expressions calculated for the perfect thick crystal cannot be expected to be valid. Calculations performed in the case of a disturbed layer on a silicon crystal have already been reported (V.G. KOHN and M.V. KOVALCHUK, 1981, Phys. Stat. Sol. (a), 64, 359-366). In the present paper the Takagi-Taupin equations have been solved in the case of a single heterostructure where the depth dependence of the strain is given by $(\Delta a/a)/(1 + \exp(z - z_I)/C)$ (see C. MALGRANGE, invited paper at this Congress). The interface is characterized by its midposition z_I and its thickness, C. The relative lattice parameter difference between epilayer and substrate is equal to $\Delta a/a$. Various situations can be obtained depending on the value of these parameters and the position of the crystal surface. Two cases are discussed here. In the first one, a heterostructure is simulated by putting the crystal surface at $z = 0$; the thickness of the epilayer is then equal to z_I and the steepness of the interface is given by C. In the second case, a disturbed surface layer is simulated by putting the surface at $z = z_I$; this corresponds to a lattice parameter which varies from the surface and stabilizes at a depth roughly equal to 2 or 3C.

The phase, the intensity of the reflected wave and the stationary wave field have been calculated in terms of the depth inside the crystal and of the angle of incidence as well as of C. The first result is that when the angle of incidence corresponds to the middle of the BRAGG peak for the substrate, the nodes and antinodes remain hooked to the atomic planes of the substrate, up to the surface and with the same periodicity. But when this angle of incidence is modified, they start drifting in a different way from that in a perfect thick crystal. Indeed, the variations of the stationary wave field, and therefore of the secondary emissions, with angle of incidence are very different from those in a perfect thick crystal. When $z = z_I$, the rocking curve is not very different from that of a perfect crystal so that an experimentator would not be alerted to the fact that the surface layer is disturbed. Nevertheless, the observed secondary emission cannot be correctly interpreted in terms of shifts of the atomic positions calculated from the perfect crystal curves; an adequate model is required for the strain. When the surface is at $z = 0$, that is when there is an epilayer of thickness z_I, oscillations occur in the expression of the Stationary Wave field for angles of incidence between the BRAGG peaks of the substrate and the epilayer. This effect, as observed by V.G. KOHN and coworkers (1982, Phys. Stat. Sol. (a), 71, 603-610), is due to interferences between waves reflected in the substrate and the epilayer. This is associated to the periodicity of the depth variations of the phase which is identical to that which occurs for a perfect thin crystal of thickness z_I (see A. AUTHIER, contributed paper to this Congress). The variations of the Stationary Wave field across the BRAGG peak of the epilayer on the other hand are quite similar to those calculated for a thin crystal of the same thickness but with a slightly different period of the fringes.

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11.7-4 SELF-CONSISTENCY AND CONSERVATION OF ENERGY IN TWO-WAVES ELECTROMAGNETIC SCATTERING. By W.A. Keller, Instituto de Fisica, Universidade Federal da Bahia, Salvador, Brasil.

The scattering of two harmonic electromagnetic plane waves by a plane of induced dipoles has been rigorously treated by means of the Hertz vector. We have shown that only a self consistent solution which takes into account cooperative effects among scatterers, is able to conserve energy. The derived complex transmission coefficients define steplike changes of amplitude and phase for both scattered waves. In two particular vibration states when the incident waves arrive at the dipole plane with the same and opposite phase, the corresponding phase-shifts display an identical behavior to that predicted by the dynamical X-ray diffraction theory. However, as the relationship between these states is derived in an exclusively analytical way, the customary use of geometrical arguments and spherical waves notion are here redudant.

11.7-5 SYNCHROTRON X-RAY WAVELENGTH TUNING APPLIED TO PENDELLÖSUNG AND STACKING FAULT FRINGE STUDIES. By A.R. Lang, G. Kowalski, A.P.W. Makepeace, H.H. Wills Physics Laboratory, University of Bristol, England and Moreton Moore, Physics Department, Royal Holloway and Bedford New College, Egham, Surrey, England.

The X-ray dynamical diffraction theory of stacking fault contrast shows that the intensity in the X-ray section topograph has 3 components, I_1 similar in form to the Pendellösung fringes in the unfaulted crystal, I_2 arising from interbranch scattering at the fault, and I_3 due to interference between I_1 and I_2 (Authier, phys. stat. sol., 1968, 27, 77-93). The component I_3 contains a term which becomes important when anomalous transmission (the Borrmann effect) is appreciable, and by which the sign of the fault vector (i.e. distinction between intrinsic and extrinsic faults) can be determined from the sign of 'first-fringe' contrast at the fault outcrop at the specimen surfaces (i.e. first fringe light or dark). In order to establish the experimental conditions needed to ensure unambiguous fault sign determination in a nearly perfect crystal, patterns have been simulated for various wavelength, absorption and Pendellösung phase conditions. Experimentally, series of synchrotron X-ray section topographs have been taken at the SRS, SERC Daresbury Laboratory, covering corresponding variations of diffraction conditions for a nearly perfect diamond crystal containing a large-area stacking fault. Particularly informative is the facility in the synchrotron case to perform a 'fine tuning' of λ by small changes of Bragg angle, so that a single cycle of the Pendellösung oscillation can be followed through. New simulation programs have been developed to cover cases of complex diffraction geometry where the fault incompletely occupies the whole 'energy-flow triangle' between $\underline{K}_o$ and $\underline{K}_g$ and these have been compared with experiment.