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Abstract. Explicit expressions are derived for the macroscopic and the internal strain in the crystals of the diamond structure with (001) surfaces subject to a stress applied from the sides parallel to the (001) direction. The numerical predictions of the surface relaxation at the ideal (001) surfaces of C, Si, Ge and α-Sn crystals are given in terms of the valence force constants already used for the description of the dynamics of the materials. The results are compared with the existing experimental observations.

1. Introduction

A peculiarity of the diamond structure is that the sites occupied by the atoms are not centrosymmetric so that the reaction of materials such as C, Si, Ge and α-Sn to an external homogeneous stress involves, apart from the usual macroscopic strain, an inner strain, which defines a mutual displacement of the constituent sublattices (Cousins 1978). The value of the inner strain has been measured in silicon (Segmüller 1963, 1964, Segmüller and Neyer 1965, d'Amour *et al* 1982), in silicon and in germanium (Cousins *et al* 1982a, b, 1987) and in diamond (Cousins *et al* 1989). It has been shown (Cousins *et al* 1987) that, while a uniaxial compressive stress is applied in the (110) direction, the inner strain near to the (001) surface significantly differs from the inner strain peculiar to the bulk. The effect has been attributed to a discrepancy between the quotient of Poisson's ratio and Young's modulus in the measured material and in the anvils used to transmit the stress. Indeed, the discrepancy produces an additional lateral stress. There exists, however, an intrinsic effect of this type which merely comes from the fact that some interactions of the atomic planes are eliminated by the existence of the surface.

The phenomenon is particularly easily tractable within a force constant model (Żabińska and Zieliński 1989, Zieliński 1990) and with the use of the surface response theory for discrete systems (Dobrzynski 1986) provided that the effective range of the interactions is not too large. A structural relaxation near to the surfaces parallel to the axis of the applied stress is expected even if no relaxation is observed in the unloaded material and no modification is introduced by the surface to the force constant values. The only condition for this strain-induced relaxation to appear is that the interactions between the atomic planes parallel to the surface of interest take in at least the second-nearest neighbour, thus assuring a spatial dispersion. The technique proposed by Żabińska and Zieliński (1989) and Zieliński (1990) seems to apply well to

diamond, silicon, germanium and α-tin crystals because they show a spatial dispersion but the effective interactions are limited to several nearest neighbours only.

Force constant models of the elastic and vibrational properties of the materials have been reviewed by Cousins (1982). A valence force potential extended to the third-nearest neighbours turned out to be satisfactory in the description of the phonon frequencies throughout the whole Brillouin zone (McMurray *et al* 1967, Tubino *et al* 1972). Weber's (1977), bond charge model which included in a simple way the electronic degrees of freedom, has confirmed the short-range character of the interactions in the crystals discussed. Also the structure of the 2×1 reconstructed (001) surfaces of Si and Ge (see, e.g., Grey *et al* 1988, Weisendanger *et al* 1990) could have been modelled with only several force constants (Appelbaum and Hamann 1978).

In more advanced *ab initio* (see, e.g., Nielsen and Martin 1985, Zandiehnadem 1990 and references therein) and semiempirical approaches (Chadi 1984, Craig and Smith 1984, 1989, 1990, Mazur and Pollmann 1989, 1990) the force constants are obtained as the respective derivatives of the lattice energy calculated by means of numerical methods. Mazur and Pollmann (1990) have shown that it is enough to consider the force constants to the sixth-nearest neighbours only so as to reproduce the bulk and the surface phonon frequencies and the structure of the reconstructed Si(001) surface well. They have also shown that the presence of the surface modifies the force constants in a surface layer extended to eight first atomic planes.

In the present work the surface relaxation of the (001) surface of C, Si, Ge and α-Sn induced by any uniaxial stress with its axis perpendicular to the (001) direction is determined within the valence potential model of McMurry *et al* (1967) and Tubino *et al* (1972). Explicit formulae are given so as to allow an interested reader to estimate quickly the extent of the phenomenon as a function of phenomenological parameters: the bulk and surface force constants and an additional surface stress. This kind of calculation offers one the possibility of assessing the expected relaxation of the surfaces in the stressed material given the values of the force constants and, therefore, to extract some additional effects such as the misfit in the elastic parameters of the sample and the anvils. On the other hand, once the relaxation is known experimentally, the adequacy of the force constant model can be checked.

The general expressions for the structure of a crystalline slab under a lateral stress are given in section 2. These expressions are then related, in section 3, to the valence force model of the diamond structure crystals given by Tubino *et al* (1972). The predicted relaxation of two possible types of the ideal (001) surfaces of C, Si, Ge and α-Sn under a uniaxial stress with its axis lying in the (001) plane is given in section 4. Section 5 presents briefly the sources of possible discrepancies between the model calculations and the results of the existing and future experiments.

2. Reaction of crystals with surfaces to external stress

Consider a crystalline slab perpendicular to the z direction and consisting of L translationally equivalent layers. Every layer generally comprises a number $K \geqslant 1$ of atomic planes. If each of the atomic planes contains atoms belonging exclusively to one single sublattice, any external homogeneous strain will only cause mutual displacements of the planes and some in-plane displacements of the atoms (Cousins 1978). It is then

convenient to introduce the following variables to describe the state of such a crystal under stress:

$$x(l) = (x_1^1(l), x_2^1(l), x_3^1(l), \ldots, x_1^K(l), x_2^K(l), x_3^K(l))$$

where $x_1^\kappa(l)$, $x_2^\kappa(l)$ and $x_3^\kappa(l)$ are the x, y and z components of the mutual displacements of the consecutive atomic planes

$$x_i^\kappa(l) = u_i^{\kappa+1}(l) - u_i^\kappa(l) \qquad \text{for } \kappa = 1, \ldots, K-1$$

$$x_i^K(l) = u_i^1(l+1) - u_i^K(l)$$

while $u_i^\kappa(l)$ is the ith component of the displacement of the κth atomic plane in the lth layer. The variables $x_i^\kappa(l)$, $i = 1, 2, 3$, are discrete analogues of local strain components ε_{13}, ε_{23}, ε_{33}, respectively.

The atomic planes themselves also undergo deformations, which can be described by the following vector:

$$\varepsilon(l) = (\varepsilon_1^1(l), \varepsilon_2^1(l)), \varepsilon_6^1(l), \ldots, \varepsilon_1^K(l), \varepsilon_2^K(l), \varepsilon_6^K(l))$$

where $\varepsilon_1^\kappa(l)$, $\varepsilon_2^\kappa(l)$ and $\varepsilon_6^\kappa(l)$ are the components of the planar strain undergone by the κth atomic plane in the lth layer. The Voigt notation is used:

$$\varepsilon_1^\kappa(l) = \varepsilon_{11}^\kappa(l) \qquad \varepsilon_2^\kappa(l) = \varepsilon_{22}^\kappa(l) \qquad \varepsilon_6^\kappa(l) = 2\varepsilon_{66}^\kappa(l).$$

If the slab is very large in the x and y directions and the external stress is applied through perfectly rigid anvils, the atomic planes are all deformed in the same way, so that the κ- and l-dependences in the above strain components can be dropped. Under such conditions and in the harmonic approximation the potential energy per unit area of the slab is

$$E = \tfrac{1}{2}\left(\varepsilon^{\mathrm{T}} \cdot \mathbf{C}\varepsilon d + 2\sum_{l=1}^{L} x^{\mathrm{T}}(l) \cdot \eta(l)\varepsilon + \sum_{l,l'=1}^{L} x^{\mathrm{T}}(l) \cdot \mathbf{h}(l, l')x(l') \right) \qquad (1)$$

where d is the thickness of the slab.

$\mathbf{C}$ is a 3×3 matrix of the elastic constants:

$$\mathbf{C} = \begin{bmatrix} c_{11} & c_{12} & c_{16} \\ c_{12} & c_{22} & c_{26} \\ c_{16} & c_{26} & c_{66} \end{bmatrix}.$$

$\mathbf{h}(l, l)$ is a matrix of the interactions of the local strain components (see Zieliński (1990) for the method of construction) and $\eta(l)$ is a coupling matrix.

When an external stress $\sigma = (\sigma_1, \sigma_2, \sigma_6)$ is applied to the slab so that its axis is perpendicular to the z direction, the state of the system is given by the following condition for the minimum of energy:

$$\frac{\partial E}{\partial \varepsilon} = \mathbf{C}\varepsilon d + \sum_{l=1}^{L} \eta^{\mathrm{T}}(l)x(l) = \sigma d \qquad (2)$$

$$\frac{\partial E}{\partial x(l)} = \eta(l)\varepsilon + \sum_{l'=1}^{L} \mathbf{h}(l, l')x(l') = s(l). \qquad (3)$$

Here $s(l)$ is a stress tending to change the separations between the atomic planes. Its most

natural source are non-compensated forces arising from the cleavage of the surfaces. In most cases the surface stress vanishes beyond a narrow subsurface zone. Equation (3) yields

$$x(l) = \sum_{l'=1}^{L} \mathbf{g}(l, l')[s(l') - \boldsymbol{\eta}(l')\varepsilon] \tag{4}$$

where $\mathbf{g}(l, l')$ is a Green function for a crystal with surfaces (Zieliński 1988, 1990). The expression for ε arises from the insertion of equation (4) into equation (2):

$$\mathbf{C}\varepsilon d + \sum_{l,l'=1}^{L} \boldsymbol{\eta}^{\mathrm{T}}(l)\, \mathbf{g}(l, l')[s(l') - \boldsymbol{\eta}(l')\varepsilon] = \sigma d. \tag{5}$$

For sufficiently thick slabs it is reasonable to assume that the strain ε is close to that in the bulk material and that $s(l)$, being zero except for a rather narrow range near the surfaces, may be neglected. Then the strain ε is calculated from equation (5) with the bulk Green function $\mathbf{G}(l, l')$ instead of the $\mathbf{g}(l, l')$ for the finite crystal and with the l-independent bulk $\boldsymbol{\eta}$ instead of $\boldsymbol{\eta}(l)$:

$$\left(\mathbf{C} - \boldsymbol{\eta}^{\mathrm{T}} \sum_{l'=-\infty}^{\infty} \mathbf{G}(0, l')\boldsymbol{\eta}\right) \varepsilon = \mathbf{C}\varepsilon = \sigma. \tag{6}$$

Substituting the strain ε from equation (6) into equation (4), one finally gets the arrangement of the atomic planes in the slab under the stress:

$$x(l) = \sum_{l'=1}^{L} \mathbf{g}(l, l')[s(l') - \boldsymbol{\eta}(l')\mathbf{C}^{-1}\sigma]. \tag{7}$$

3. Application to the valence force model

Valence potential models relate the lattice energy to variations in the bond lengths and bond angles. The appropriate transformation allows one to express this energy in terms of the variables of interest, i.e. ε and $x(l)$ as defined in the previous section. In the case of the (001) surface of the diamond structure crystals there are two translationally inequivalent atomic planes so that $K = 2$. McMurry *et al* (1967) and Tubino *et al* (1972) have introduced the following valence force constants: K_R for the bond stretching F_R for the interactions of the stretchings of the bonds having a common apex, H_Λ for the bending of the angles between bonds of common apex, $F_{R\Lambda}$ for the interaction of the angles with the stretching of the adjacent bonds, $F_{\Lambda'}$ for the interaction of two angles having one apex and one bond in common and $F_{\Lambda''}$ for the interactions of coplanar angles whose apexes are separated by a bond common to both angles. Here, all the force constants are in units of energy per square ångström. Below the coefficients $\mathbf{C}$, $\boldsymbol{\eta}(l)$ and $h(l, l')$ of equation (1) are given in terms of the valence force constants:

$$\begin{aligned}
c_{11}/a^2 &= c_{22}/a^2 = \tfrac{1}{12}K_R + \tfrac{1}{3}F_R + \tfrac{16}{9}H_\Lambda - \tfrac{32}{9}F_{\Lambda'} + \tfrac{32}{9}F_{\Lambda''} \\
c_{12}/a^2 &= c_{21}/a^2 = \tfrac{1}{12}K_R + \tfrac{1}{3}F_R - \tfrac{8}{9}H_\Lambda + \tfrac{16}{9}F_{\Lambda'} - \tfrac{16}{9}F_{\Lambda''} \\
c_{66}/a^2 &= \tfrac{1}{12}K_R - \tfrac{1}{6}F_R + (8/3\sqrt{6})F_{R\Lambda} + \tfrac{8}{9}H_\Lambda + \tfrac{16}{9}F_{\Lambda''} \\
c_{16} &= c_{61} = c_{26} = c_{62} = 0.
\end{aligned} \tag{8}$$

a is the cubic lattice parameter. Since in the cubic crystallographic system $c_{12} = c_{13} = c_{23}$ and $c_{66} = c_{44} = c_{55}$, the above list exhausts all the different elastic constants.

It follows from the symmetry of the diamond structure that the strain components ε_1, ε_2 and ε_6 are only coupled to $x_3^1(l)$ and $x_3^2(l)$. The non-zero coupling parameters can be, therefore, grouped in a 2×3 matrix $\boldsymbol{\eta}$ whose elements η_{ij}, $i = 1, 2, j = 1, 2, 6$, in the bulk (far from the surfaces) are l independent and read

$$\eta_{11}/a = \tfrac{1}{6}K_R + F_R - \tfrac{16}{9}H_\Lambda + \tfrac{32}{9}F_{\Lambda'} - \tfrac{32}{3}F_{\Lambda''}$$

$$\eta_{16}/a = -\tfrac{1}{6}K_R + \tfrac{1}{3}F_R + (8/3\sqrt{6})F_{R\Lambda} + \tfrac{32}{9}H_\Lambda + \tfrac{64}{9}F_{\Lambda''} \qquad (9)$$

$$\eta_{12} = \eta_{21} = \eta_{22} = \eta_{11} \qquad \eta_{26} = -\eta_{16}.$$

The relationship $\eta_{26} = -\eta_{16}$ means that under a shear ε_6 the distances $x_3^1(l)$ and $x_3^2(l)$ are changed so that $x_3^1(l) = -x_3^2(l)$, which corresponds to a pure inner strain in Cousins' (1978) theory.

Owing to the high symmetry of the (001) direction the lateral displacements $x_1^1(l)$, $x_2^1(l)$, $x_1^2(l)$ and $x_2^2(l)$ are decoupled from $x_3^1(l)$ and $x_3^2(l)$. Since only the latter are affected by the applied strain ε_i, $i = 1, 2, 6$, it is enough to consider a 2×2 matrix $\mathbf{h}(l, l')$:

$$h_{11}(l, l) = h_{22}(l, l) = \tfrac{2}{3}K_R + \tfrac{4}{3}F_R - (64/3\sqrt{6})F_{R\Lambda} + \tfrac{320}{9}H_\Lambda - \tfrac{128}{3}F_{\Lambda'} + 64F_{\Lambda''}$$

$$h_{12}(l, l) = h_{21}(l, l) = h_{12}(l, l-1) = h_{21}(l, l+1) \qquad (10)$$

$$= \tfrac{4}{3}F_R + (32/3\sqrt{6})F_{R\Lambda} + \tfrac{32}{9}H_\Lambda - \tfrac{64}{3}F_{\Lambda'} + \tfrac{64}{9}F_{\Lambda''}$$

$$h_{11}(l, l+1) = h_{11}(l, l-1) = h_{22}(l, l+1) = h_{22}(l, l-1) = \tfrac{32}{9}F_{\Lambda''}.$$

All the other elements $h_{ij}(l, l')$ vanish.

The force constants in equations (8)–(10) should all be given in units of energy per square ångström. Consequently, the parameters $F_{R\Lambda}$, H_Λ, $F_{\Lambda'}$ and $F_{\Lambda''}$ of Tubino *et al* (1972) have to be replaced by $F_{R\Lambda}/a$, H_Λ/a^2, $F_{\Lambda'}/a^2$ and $F_{\Lambda''}/a^2$, respectively.

Since the diamond structure comprises two inequivalent atomic layers perpendicular to the z direction, there exist two different ways of cleaving the ideal (001) surface. The topmost atomic layer may then be located either at $z = 0$ or at $z = \tfrac{1}{4}$ with respect to the origin of the unit cell. (Both kinds of surface are related with one another through a $\pi/2$ rotation about the z axis.) Correspondingly, given the external stress σ we shall consider the relaxation of the surface of the first kind as the succession $x_3^1(1), x_3^2(1), x_3^1(2), x_3^2(2), \ldots$ and the relaxation of the surface of the second kind as $x_3^2(1), x_3^1(2), x_3^2(2), x_3^1(3), \ldots$ An analogous distinction of the two kinds of surface can be made at the other periphery of the slab, i.e. for l close to L.

The presence of the surfaces results in a modification of the elements of the energy matrix $\mathbf{h}(l, l')$ (see equation (1)) for l and l' close either to unity or to L compared with the bulk values of these elements given in equation (10). In the present calculations the surfaces are treated as ideal in the sense that their existence only eliminates some force constants, whereas all the remaining force constants preserve their values peculiar to the bulk. The rule of elimination applied here is the following: whenever a bond is crossed by the surface plane (assumed to be infinitesimally shifted outwards with respect to the topmost atomic plane), all the contributions to the lattice energy are dropped if they involve a variation in the length of this bond or a variation in an angle that the bond is a side of. The rule can be immediately expressed in terms of the valence variables, i.e. the bond lengths and bond angles. After the transformation to the variables of interest

$x^1_3(l)$, $x^2_3(l)$ and ε_j one finds that in the case of the first kind of surface at $l = 1$ the elements of the cleavage operator given by

$$V^1_{11}(1, 1) = -[(32/3\sqrt{6})F_{R\Lambda} + \tfrac{32}{9}H_\Lambda - \tfrac{64}{9}F_{\Lambda'} + \tfrac{64}{9}F_{\Lambda''}]$$
$$V^1_{12}(1, 1) = V^1_{21}(1, 1) = -\tfrac{32}{9}F_{\Lambda''}$$

(11)

have to be added to the respective elements $h_{11}(1, 1)$, $h_{12}(1, 1)$ and $h_{21}(1, 1)$ implied by equation (10).

Similarly, for the second kind of surface at $l = 1$ the cleavage operator reads

$$V^2_{11}(1, 1) = -h_{11}(l, l) \qquad V^2_{12}(1, 1) = V^2_{21}(1, 1) = -h_{12}(l, l)$$
$$V^2_{22}(1, 1) = V^1_{11}(1, 1) \qquad V^2_{21}(1, 2) = V^2_{12}(2, 1) = V^1_{12}(1, 1).$$

(12)

One should note that the above cleavage operators (equations (11) and (12)) do not follow the definition of the cleavage operator appropriate to the Born and von Karman force constant model (Zieliński 1988).

The matrix $\boldsymbol{\eta}(l)$ also differs from that given in equation (9) when l is close to unity. Correspondingly, for the first kind of surface one has

$$\eta^1_{11}(1) = \eta^1_{12}(1) = \eta_{11} - \tfrac{1}{3}F_R - (4/3\sqrt{6})F_{R\Lambda} + \tfrac{4}{9}H_\Lambda - \tfrac{16}{9}F_{\Lambda'} + \tfrac{8}{9}F_{\Lambda''}$$
$$\eta^1_{16}(1) = \eta_{16} - \tfrac{1}{3}F_R$$

(13)

$$\eta^1_{21}(1) = \eta^1_{22}(1) = \eta_{11} + \tfrac{8}{9}F_{\Lambda''}.$$

The remaining elements $\eta_{ij}(l)$ are equal to η_{ij} of equation (9). For the second kind of surface

$$\eta^2_{1j}(1) = 0 \qquad \text{for } j = 1, 2, 6$$
$$\eta^2_{21}(1) = \eta^2_{22}(1) = \eta^1_{11}(1) \qquad \eta^2_{26}(1) = \eta_{26} + \tfrac{1}{3}F_R$$

(14)

$$\eta^2_{11}(2) = \eta^2_{12}(2) = \eta_{11} + \tfrac{8}{9}F_{\Lambda''}.$$

The cleavage operators $\mathbf{V}(l, l')$ and the coupling matrices $\boldsymbol{\eta}(l)$ at the other surface of the slab can be easily obtained from equations (11)–(14) by the appropriate replacement of indices.

4. Surface relaxation

The form of the bulk energy matrix (equation (10)) allows one to express the bulk static Green function $G_{\alpha\beta}(l, l')$ directly by the elements of the Green function $G^0(m, m')$ for a system of identical atomic planes with interactions extended to the third-nearest neighbours (Zieliński 1988):

$$G_{\alpha\beta}(l, l') = G^0(2l + \alpha - 2, 2l' + \beta - 2)$$

where

$$G^0(m, m') = (1/h_{12}(1, 2))[z_1^{|m - m'|+2}/(z_1^2 - 1)(z_1 - z_2)(z_1 - z_2^{-1})$$
$$+ z_2^{|m - m'|+2}/(z_2^2 - 1)(z_2 - z_1)(z_2 - z_1^{-1})].$$

(15)

The quantities $z_i, i = 1, 2, |z_i| < 1$, which either are both real or have $z_1 = z_2^*$, define the

Table 1. Parameters z_1 and z_2 of the bulk Green function (equation (15)) for C, Si, Ge and α-Sn crystals.

	$\mathrm{Re}(z_1)$	$\mathrm{Im}(z_1)$	$\mathrm{Re}(z_2)$	$\mathrm{Im}(z_2)$
C	−0.140	0	−0.072	0
Si	−0.068	0.074	−0.068	−0.074
Ge	−0.073	0.082	−0.073	−0.082
α-Sn	−0.104	0.017	−0.104	−0.017

spatial behaviour of the deformation caused to the crystal by a body force applied to atomic plane m. The specific expression for z_1 and z_2 in terms of the elements of the energy matrix $\mathbf{h}(l, l')$ has been given by Zieliński (1988). Table 1 shows the values of z_1 and z_2 for the crystals C, Si, Ge and α-Sn. The negative values of $\mathrm{Re}(z_1)$ and $\mathrm{Re}(z_2)$ mean that the asymptotic relaxation in all the considered crystals has an alternating character (Allan and Lannoo 1988). The wave of the alternation is incommensurate with the lattice in Si, Ge and α-Sn, the wavenumber being equal to $\arg(z_1)$.

The rate of the spatial relaxation of the deformation is determined by the greatest modulus $|z_i|$. In the present model, $|z_i| \simeq 0.1$ except for diamond where $|z_1| = 0.140$. Thus, the diamond crystal shows the slowest spatial relaxation.

Using the bulk Green function (equation (15)) and the cleavage operators for both kinds of surface (equations (11) and (12)), one can obtain the corresponding Green functions $g(l, l')$ for the crystal with surface (see Dobrzynski (1986) and Zieliński (1990) for details of the calculation). The limited spatial range of the cleavage operators (equations (11) and (12)) and the relatively small values of $|z_i|$ indicate that the surface relaxation will extend to several subsurface atomic layers only. That is why, when considering the surface relaxation under a stress σ (equation (7)), one can put $L \rightarrow \infty$ even for fairly thin slabs.

The reaction of the ideal (001) surfaces of the crystals C, Si, Ge and α-Sn to a lateral uniaxial stress is shown in figures 1, 2, 3 and 4, respectively. The quality 'ideal' means here that no variation has been introduced into the force constants near the surfaces apart from those implied by equation (11)–(14). Further, no surface stress $s(l)$ has been taken into account. The angle between the axis of the external stress with the (100) crystallographic direction has been denoted by φ. (In the experiments of Cousins *et al* (1982a,b, 1987, 1989), $\varphi = \pi/4$.) The full curves with crosses and the full curves in figures 1–4 show the changes in the first and the second interlayer spacings, respectively, compared with the corresponding changes in the bulk crystal indicated by the chain curves and broken curves, respectively. The value of the external compressive stress has been set at 1 GPa for all angles.

5. Discussion

Surface relaxation under a lateral stress has been observed by Cousins *et al* (1987) in silicon and germanium as an artefact in a measurement of the bulk internal strain. The latter quantity is proportional to $x^2(l) - x^1(l)$. According to Cousins *et al* (1987) the relative difference between the internal strain near the surface and that in the bulk is about 30%. However, to the present author's knowledge there are no experiments specifically aimed at the study of the surfaces under such a stress. In the present
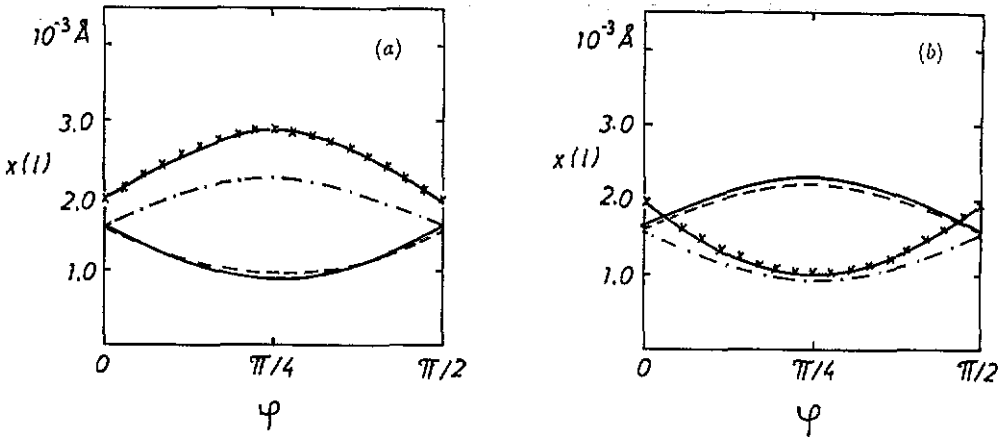
Figure 1. (a) Variations in the first $x^1(1)$ (— * —) and second $x^2(1)$ (——) interlayer distances at the (001) surface of type 1 in diamond under a uniaxial stress of 1 GPa with its axis making an angle φ with the direction (100). The corresponding variations in the interlayer distances $x^1(l)$ (— · —) and $x^2(l)$ (– – –) in the bulk are also shown. (b) Variations in the first $x^2(1)$ (— * —) and second $x^1(2)$ (——) interlayer distances at the (001) surface of type 2 in diamond under a uniaxial stress of 1 GPa with its axis making an angle φ with the direction (100). The corresponding variations in the interlayer distances $x^2(l)$ (— · —) and $x^1(l)$ (– – –) in the bulk are also shown.
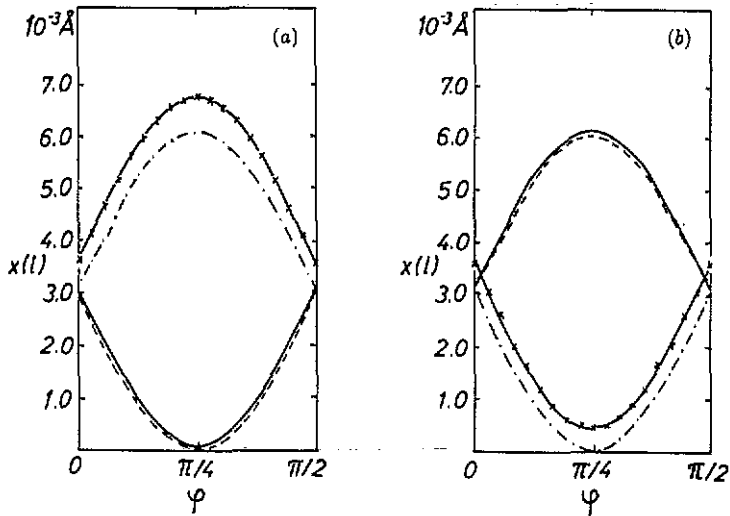

Figure 2. Same as for figure 1 but for the (001) surface of Si.

calculations based on the force constant model of Tubino *et al* (1972) the relative difference of the surface and the bulk internal strain slightly exceeds about 10% for Si and Ge and is about 60% in the case of the surface of type 1 in diamond. In all cases, however, the effect quickly diminishes with increasing depth into the crystal owing to small values of $|z_i|$, whereas the effect observed by Cousins *et al* must have taken in more atomic planes so that it is perceivable in a diffraction experiment.
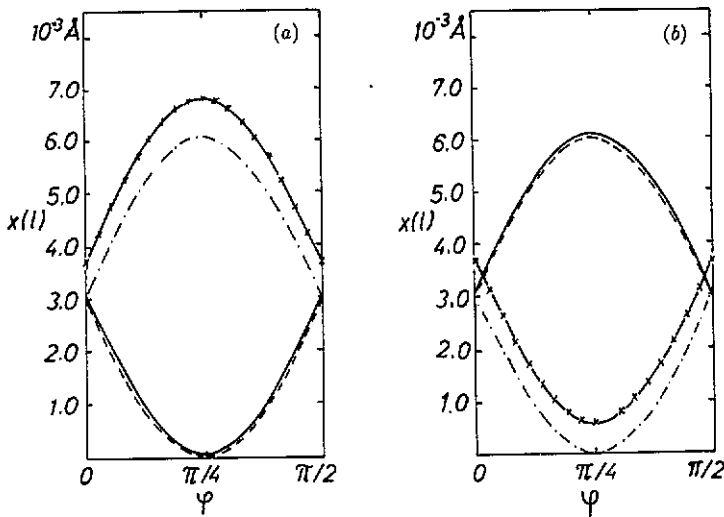
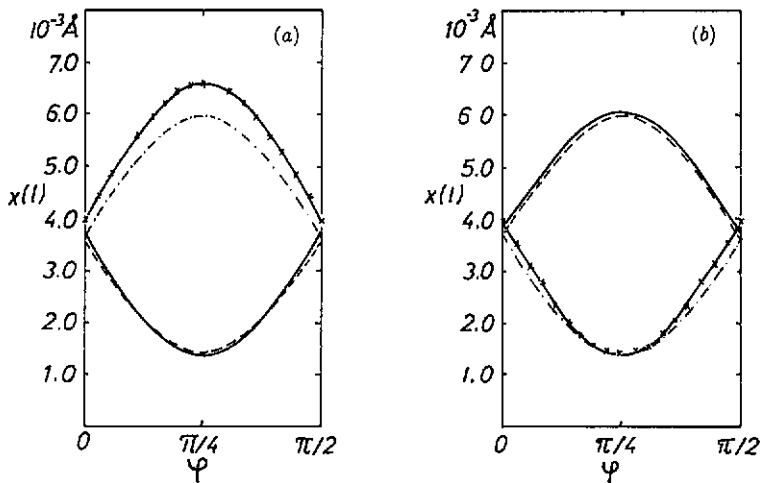**Figure 3.** Same as for figure 1 but for the (001) surface of Ge.

Figure 4. Same as for figure 1 but for the (001) surface of α-Sn.

The reasons for possible discrepancies between the present calculations and experimental results are, apart from those raised by Cousins *et al* (1987), the following. Firstly, even well prepared (001) surfaces of diamond structure are stepped (see, e.g., Kawamura *et al* 1988, Weisendanger *et al* 1990) so that there exists a surface zone where the 'topmost atomic layer' lies at different levels. Secondly, the surfaces considered are 2 × 1 reconstructed, which may cause a variation in the surface force constants. Finally, even though the surfaces were perfectly flat, the force constant model, which accounts for bulk dynamical properties well, may be inadequate close to the surface. In particular the polarization of the bonds near to the surface may influence not only the value but also the spatial extent of the parameters of the harmonic interactions (Mazur and

Pollmann 1989). The results given in section 4 should, therefore, be treated as a starting point in a generalization of the model of Tubino *et al* (1972) to systems with surfaces. It seems that experiments aimed at the study of the influence of the lateral stress on the structure of surfaces will soon provide indications on how such an improvement can be achieved.

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