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Moiré Fringes and/or Translation-Fault Fringes?

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Abstract

Interference fringes on transmission topographs of crystals with an implanted amorphous layer are, among others, attributed to the moiré or the translation-fault effect. This discussion is reconsidered in the frame of the theory of a perfect bicrystal extended to a deformed one. It is shown that translation-fault fringes have the same properties as moiré fringes and that it is not necessary to introduce translation-fault fringes as a new diffraction phenomenon.

1. Introduction

The investigation of X-ray interference phenomena is an important tool to characterize implanted layers in silicon crystals. Damage build up due to implantation has been studied by Milita & Servidori (1995). Strain gradient profiles in silicon implanted with high-energy α particles were evaluated by Wieteska & Wierzchowski (1995). Moiré fringes observed on X-ray diffraction topographs of SIMOX samples (separation by implantation of oxygen) have revealed lattice mismatches of the order of 10^{-7} between the top silicon layer and the substrate (Jiang, Shimura & Rozgonyi, 1990; Ohler, Prieur & Härtwig, 1996).

Interference fringes on transmission X-ray diffraction topographs of crystals with an implanted layer can be related to different generation processes. When they are due to spatial variations of layer thicknesses or the *Pendellösung* length, they are most often called *Pendellösung* fringes. Moiré fringes are formed by the superposition of two crystal lattices of slightly different orientation or with slightly different lattice parameters. Translation-fault fringes, introduced by Bonse & Hart (1969), image the spatial variation of the displacement field between the two parts of a bicrystal. For other types of interference fringes, see for example the work of Wieteska & Wierzchowski (1995).

Simon & Authier (1968) observed interference fringes on X-ray topographs of ion-implanted silicon and interpreted them as moiré fringes. Similar samples, investigated by Bonse, Hart & Schwuttke (1969), lead to comparable results but the fringes were attributed to a translation fault between the silicon layer on top of a buried amorphous layer and the substrate.

The aim of the present article is to solve this obvious contradiction. This seems important as in recent studies of implanted layers some confusion is found on the distinction between moiré fringes and translation-fault fringes. This solution may help the development of X-ray interferometry and crystal device characterization.

2. X-ray diffraction by a perfect bicrystal

A perfect bicrystal is produced from a single-crystal plate with parallel surfaces by a separation of one part from the other. The two parts can then be translated relative to each other by a rigid-body translation (i), which results in a stacking fault. It also leads to the formation of a gap when the translation has a component perpendicular to the separation plane. The lattice of one crystal can further be rotated with respect to the other (ii) and/or the lattice parameter(s) of one of the two crystals can be modified (iii).

A stacking fault that is not parallel to the crystal surface can lead to interference fringes on X-ray topographs (Authier, 1968; Wierzchowski & Moore, 1996). When the stacking-fault plane is parallel to the surface, the bicrystal shows translation symmetry in this direction. In this case, a rigid-body translation (i) between the two plates cannot give rise to intensity oscillations on an X-ray topograph. Cases (ii) and (iii) lead to different reciprocal-lattice vectors $\mathbf{H}$ and $\mathbf{H}'$ in the first and the second part of the bicrystal. However, intensity variation on an X-ray topograph, necessarily related to a break in the translation symmetry of the sample, are only expected if the component of $\Delta\mathbf{H} = \mathbf{H}'-\mathbf{H}$ parallel to the sample surface, $\Delta\mathbf{H}_{\parallel}$, does not vanish (Ohler, Prieur & Härtwig, 1996).

For many implanted layers, and also for the samples studied by Simon & Authier (1968) and Bonse, Hart & Schwuttke (1969), the interface plane between the two crystalline parts of the bicrystal is highly parallel to the crystal surfaces. Therefore, interference fringes on X-ray topographs of such bicrystals must be attributed to a reciprocal-lattice-vector difference between the two crystal plates and thus to the moiré effect.

Let $\mathbf{u}(\mathbf{r})$ be the displacement of the atoms in the second crystal plate relative to those in the first plate. $\mathbf{u}(\mathbf{r})$ contains rigid-body translation, rotation and lattice-parameter differences. For two perfect plates with different but constant reciprocal-lattice vectors $\mathbf{H}$ and $\mathbf{H}'$, $\mathbf{u}(\mathbf{r})$ is a linear function in $\mathbf{r}$. For the most general case, the Takagi equations (Takagi, 1962, 1969) have to be used to describe the diffraction by a deformed bicrystal (*e.g.* Wieteska & Wierzchowski, 1995). In the following, the X-ray diffraction by a perfect bicrystal is formulated in terms of the deformed crystal theory, using the concept of the local reciprocal lattice. With an eye on later generalization, the effect of the displacement field $\mathbf{u}(\mathbf{r})$ can then be accounted for in the following way:

$$\begin{aligned}\chi'_H &= \chi_H \exp\{2\pi i\mathbf{H}\cdot[\mathbf{r}-\mathbf{u}(\mathbf{r})]\}\\ &= \chi_H \exp\Big(2\pi i\{\mathbf{H}\cdot[\mathbf{r}-\mathbf{u}(\mathbf{r}_0)]\\ &\quad + \Delta\mathbf{H}(\mathbf{r}_0)\cdot(\mathbf{r}-\mathbf{r}_0)\}\Big). \qquad (1)\end{aligned}$$

$\Delta\mathbf{H}(\mathbf{r}_0) = -\mathrm{grad}[\mathbf{H}\cdot\mathbf{u}(\mathbf{r})]|_{\mathbf{r}=\mathbf{r}_0}$ is the reciprocal-lattice-vector difference between the two crystals at some arbitrary point $\mathbf{r}_0$ in the second crystal. The χ_H are the Fourier components of the dielectric susceptibilities of the first and second crystals. The term $\mathbf{H}\cdot\mathbf{u}(\mathbf{r}) + \Delta\mathbf{H}(\mathbf{r}_0)\cdot\mathbf{r}_0$ results in a constant phase factor for the susceptibilities χ'_H of the second crystal while $[\mathbf{H} + \Delta\mathbf{H}(\mathbf{r}_0)]\cdot\mathbf{r}$ describes the excitation of new tie points and the creation of new wave fields in the second crystal (Polcarova, 1978, 1980). When the intensity distribution at the exit surface of the bicrystal is calculated, all waves created in the second crystal have to be summed. The result for a gapped bicrystal with different reciprocal-lattice vectors is given by Yoshimura (1996). These expressions can be rewritten for both the forward-diffracted (0) and the diffracted beam (H) as

$$I_{0,H} = A_{0,H} + B_{0,H}\cos\{2\pi[\Delta\mathbf{H}(\mathbf{r}_0)\cdot(\mathbf{r}-\mathbf{r}_0)]\}. \qquad (2)$$

$A_{0,H}$ and $B_{0,H}$ are functions of the tie points excited in both crystal parts and depend also on the gap thickness. It has been shown by Yoshimura (1991) that the gap thickness plays an important role only when it is comparable to or larger than the *Pendellösung* length. Thus, to influence the contrast on an X-ray topograph, its variations must be on this scale. For the samples studied by Bonse, Hart & Schwuttke (1969), for example, the gap thickness is of the order of a fraction of a micrometre and thus much smaller than the *Pendellösung* length.

The position vectors $\mathbf{r}$ and $\mathbf{r}_0$ in (2) can be chosen to be two observation points on the exit surface of the crystal. The diffracted intensity then cycles through an oscillation between $\mathbf{r}$ and $\mathbf{r}_0$ whenever the function $N(\mathbf{r},\mathbf{r}_0) = \Delta\mathbf{H}(\mathbf{r}_0)\cdot(\mathbf{r}-\mathbf{r}_0)$ equals an integer. These intensity oscillations, related to a reciprocal-lattice-vector difference between the two crystals, are called moiré fringes. The properties of moiré fringes (interfringe distance, fringe direction, contrast) can be derived from (2).

3. Description of the deformed bicrystal

Bonse, Hart & Schwuttke (1969) studied silicon layers on top of buried amorphous layers produced by ion implantation. As no fringes were observed on symmetrical transmission topographs, the deformation field of the layer, $\mathbf{u}(\mathbf{r})$, was assumed to be parallel to the surface normal, $\mathbf{u}(\mathbf{r}) \parallel \mathbf{n}$. It has been shown before that no intensity oscillations can be expected on an X-ray topograph if this deformation field is constant or linear in $\mathbf{r}$. However, a nonlinear $\mathbf{u}(\mathbf{r})$ necessarily means that the shot-through layer must be considered as a deformed crystal and must be treated in an adequate formalism.

Under certain conditions, the theory of the X-ray diffraction by a perfect crystal can be extended to the deformed crystal on a local scale (Härtwig, Holy, Kittner, Kubena & Lerche, 1988). The same is possible for the deformed bicrystal with a nonlinear deformation field $\mathbf{u}(\mathbf{r})$. Therefore, $\Delta\mathbf{H}(\mathbf{r})$ must be approximately constant over the effective area of the crystal (Kubena & Holy, 1983). In this case, (2) holds on a local scale and $A_{0,H}$ and $B_{0,H}$ depend on the locally excited tie points. $\mathbf{N}(\mathbf{r},\mathbf{r}_0)$ must then be calculated in a cummulative manner:

$$\begin{aligned}N(\mathbf{r},\mathbf{r}_0) &= \int_{\mathbf{r}_0}^{\mathbf{r}} \Delta\mathbf{H}(\mathbf{u})\,\mathrm{d}\mathbf{r}'\\ &= \int_{\mathbf{r}_0}^{\mathbf{r}} \mathrm{grad}[\mathbf{H}\cdot\mathbf{u}(\mathbf{r}')]\,\mathrm{d}\mathbf{r}'\\ &= \mathbf{H}\cdot\mathbf{u}(\mathbf{r}) - \mathbf{H}\cdot\mathbf{u}(\mathbf{r}_0)\end{aligned}$$

and is not $\Delta\mathbf{H}(\mathbf{r})\cdot\mathbf{r}$ as proposed by Simon & Authier (1968). Thus, the geometry of moiré fringes (fringe direction and fringe distance) is a map of $\mathbf{H}\cdot\mathbf{u}(\mathbf{r})$. However, for the intensity profile, the excited tie points in both crystal plates have to be considered.

4. Translation-fault fringes and moiré fringes

According to Bonse & Hart (1969), the properties attributed to translation-fault fringes can be summarized as follows:

(i) they are a map of $\mathbf{H}\cdot\mathbf{u}(\mathbf{r})$ of the relative displacement field between two crystal plates, $\mathbf{u}(\mathbf{r})$;

(ii) they result in the same fringe pattern for different diffraction vectors when the projection of the diffraction vector on the surface normal, $\mathbf{H}\cdot\mathbf{n}$, is the same;

(iii) they show contrast reversal for reversed beam-entrance and beam-exit surfaces.

It has been shown before that (i) is a property of moiré fringes as long as the local application of the theory of the perfect bicrystal to the deformed bicrystal is valid. In consequence, (ii) is also expected for moiré fringes when $\mathbf{u}(\mathbf{r})$ is parallel to the surface normal. The topographs presented by Bonse, Hart & Schwuttke (1969) were recorded under the conditions of anomalous transmission on a bicrystal composed of a thin and a thick crystal plate. When the complete solution for the bicrystal, as presented by Polcarova (1978), for example, is specified in this special case, it is seen that moiré fringes also show contrast reversal (iii) under these conditions (Ohler & Härtwig, 1997) and this effect cannot uniquely be attributed to translation-fault fringes.

In the frame of the local application of the perfect bicrystal theory to the deformed bicrystal, the intensity at any observation point on the exit surface depends on the tie points selected in both crystal plates. Careful recalculation of the derivation by Bonse & Hart (1969) and comparison with the results obtained by Polcarova (1978) shows that the theory presented by Bonse & Hart (1969) holds for the special case where the difference between the tie points excited in the first and in the second crystal can be neglected, namely that $\Lambda_0 \Delta\mathbf{H} \cdot \mathbf{s}_{0,H}/\gamma_{0,H}$ is very small (Λ_0 is the *Pendellösung* length, $\mathbf{s}_{0,H}$ are the unit vectors in the forward-diffracted and the diffracted direction, respectively, and $\gamma_{0,H}$ are the corresponding direction cosines). This is exactly fulfilled when $\Delta\mathbf{H}$ is perpendicular to the diffraction plane.

Finally, Bonse, Hart & Schwuttke (1969) discuss moiré fringes on a pseudomorphic structure ($\Delta\mathbf{H}_{\|} = 0$) to demonstrate that the fringes they observed are of a new type and not moiré fringes (Fig. 8 of their article). It was shown before that no fringes are expected on an X-ray topograph of such a bicrystal.

5. Discussion and conclusions

It has been shown that under the following special conditions moiré fringes have the properties that were exclusively attributed to translation-fault fringes by Bonse, Hart & Schwuttke (1969):

(i) the displacement field between the two crystals is normal to the crystal surface (no fringes observed on symmetrical transmission topographs);

(ii) the topograph is recorded under the conditions of anomalous transmission on a bicrystal composed of a thin layer and a thick substrate (contrast reversal for reversed beam-entrance and beam-exit surfaces).

For a linear displacement field between the two parts of a bicrystal, both crystal plates are perfect and X-ray diffraction on such a structure can be described with the perfect-crystal theory. When the displacement field is not linear but grad$[\mathbf{H} \cdot \mathbf{u}(\mathbf{r})]$ varies on a scale larger than the effective area of the crystal, the same formalism can be used on a local scale. In cases when this approximation is not valid, the complete Takagi formalism has to be employed.

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