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On the origin of HOLZ lines splitting near interfaces: multislice simulation of CBED patterns

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Abstract Splitting of HOLZ lines on CBED patterns is systematically observed at the proximity of interfaces and prevents local strain measurements by monitoring of line shifts. It was previously suggested that such splitting occurs due to interface-strain relaxation in thin TEM lamella. Here we confirm this model by dynamical simulation of CBED patterns using the multislice algorithm.

Keywords CBED, strain analysis, line splitting, dynamical simulation, multislice

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Recent developments in semiconductor devices showed that CMOS transistor performance could be considerably improved by introducing mechanical stress in silicon [1,2]. To develop and stabilize finite element method calculation, and finally to optimize the transistor performance, it is necessary to have a technique capable to measure the strain distribution in the transistor channel region with an accuracy below 1% and with nanometer resolution.

One of the most promising techniques is the Convergent Beam Electron Diffraction (CBED) method [3–7], because higher order Laue zone (HOLZ) line positions shift sensitively with lattice parameter changes. Recently developed software [8] provides the possibility to extract the strain tensor semi-automatically from the CBED pattern of silicon and thus opens this generally very time-consuming method to the industry. Based on a line detection algorithm and the kinematical theory, the software utilizes the ⟨230⟩ Si zone at 200 kV. A reference pattern is taken deep in the Si in order to observe a relative shift of HOLZ lines in the region of interest. But as seen in Fig. 1, while the pattern obtained at 500 nm depth below the interface corresponds well to the expected ⟨230⟩ Si CBED pattern and represents sharp lines, in the region closer to the interface, i.e. in the region defining the transistor properties, broadening and

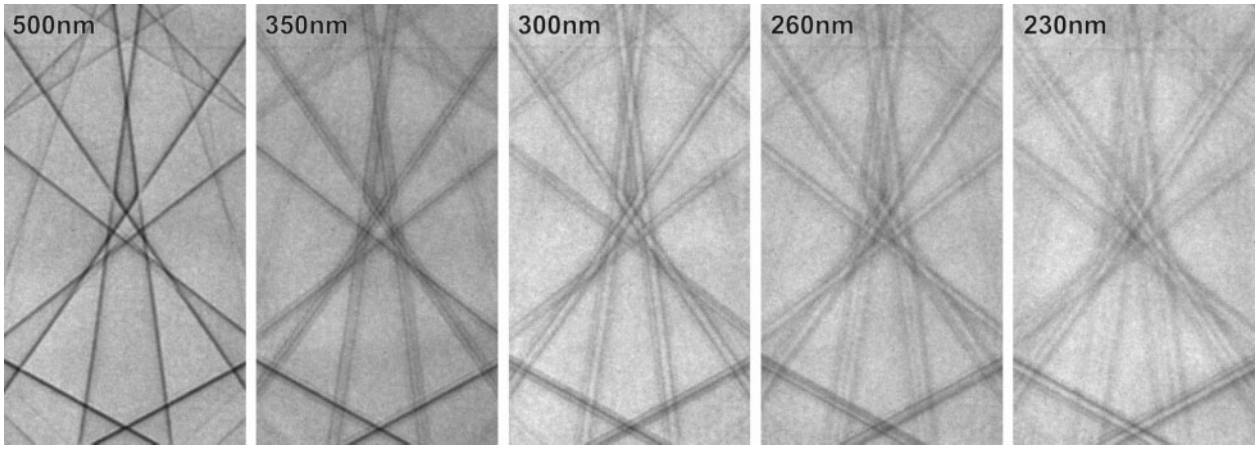

Fig. 1 A stack of Si <230> CBED patterns, obtained at the positions sequentially approaching the interface (left to right, distance to interface is indicated), shows the evolution of the HOLZ lines splitting.

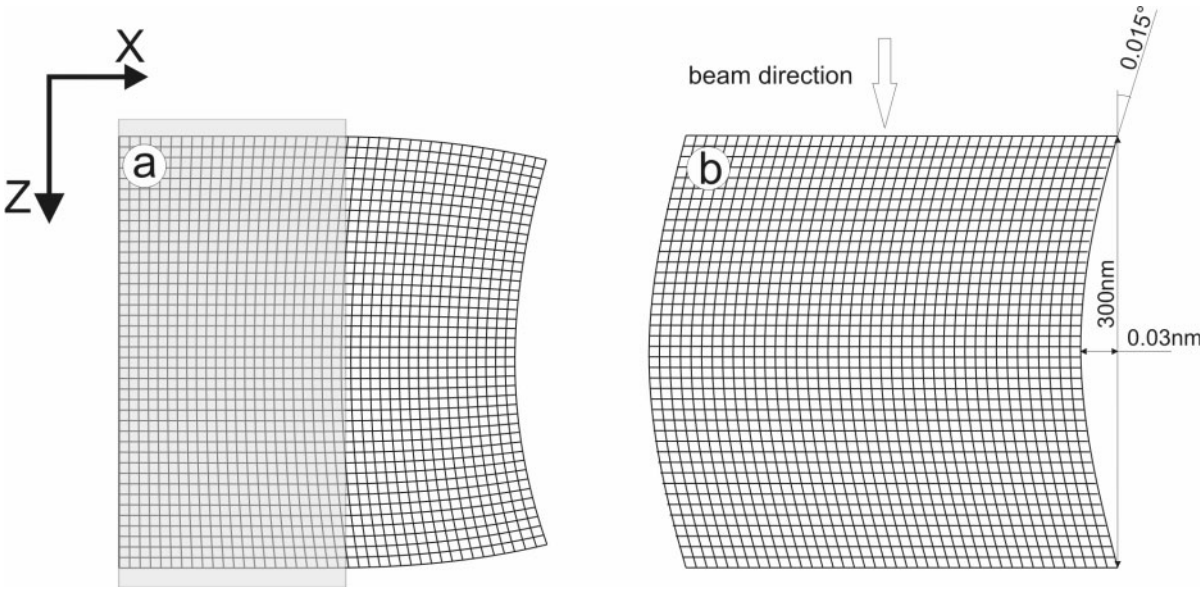

Fig. 2 (a) Scheme of a strain field near an interface after thin lamella relaxation; (b) scheme of a strain field utilized in the simulation. The $\partial e_{zz}/\partial x$ component of strain gradient is excluded; actual values of applied displacements are indicated. The shaded rectangle at (a) indicates the region where the $\partial e_{zz}/\partial x$ component of strain gradient is negligible, so that model (b) is correct for this region.

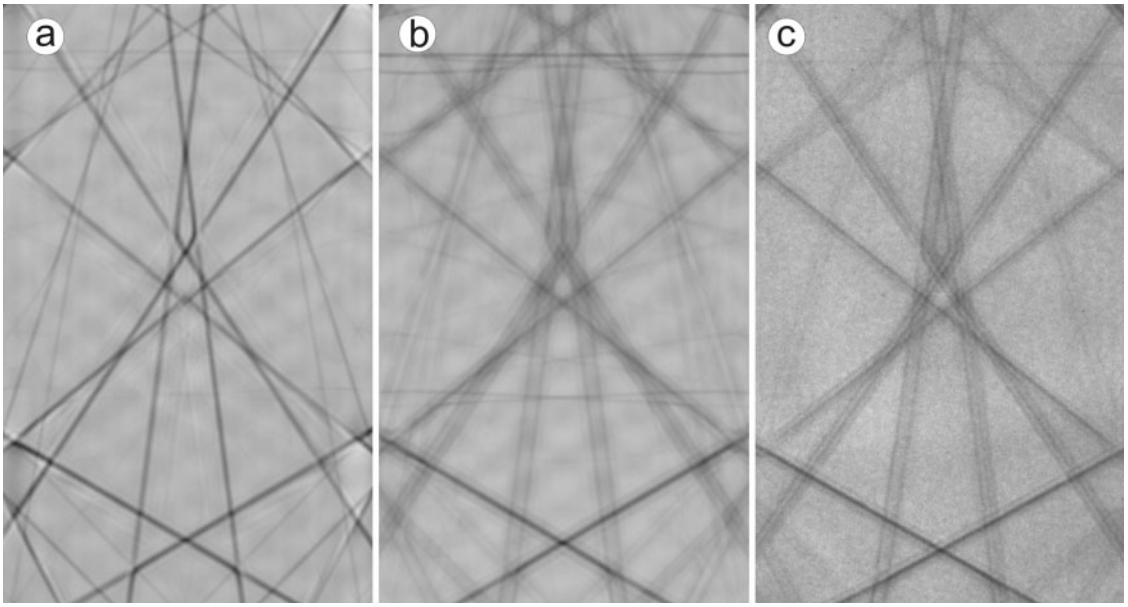

Fig. 3 Central parts of the 000 CBED disks for Si <230> zone at 200 kV: (a) simulated pattern for a perfect crystal; (b) simulated pattern for bended crystal in accordance to Fig. 2b; (c) experimental image (identical to Fig. 1, 350 nm) at similar conditions (high tension deviates slightly from the nominal 200 kV, 300 nm thickness, measured by thickness fringes of the CBED pattern).

splitting-like effects are observed, which invalidate the usage of line-shift based detection algorithm.

Observing that the splitting effect did not appear near a free Si but near a covered Si surface, Banhart [9] explained the splitting by lattice bending caused by strain relaxation in the thin TEM lamella. The strain originated from the thermal expansion coefficient difference between Si and the cover layer. Later this model was discussed by a number of authors [10,11]; however, no proof has been provided so far. Here we apply the multislice algorithm in order to simulate the HOLZ lines splitting effect in a bended crystal.

The multislice method is widely and successfully used for the calculation of scattering of fast electrons for the purpose of HRTEM image simulation. Recently we demonstrated that this method is also capable of calculating HOLZ lines in CBED patterns [12,13]. The advantage of the multislice method is that it does not require an approximation of slowly varying crystal parameters and thus it is a perfect tool

for simulation of electron scattering by strained materials. So far the existing algorithm does not allow simulation of any strain field with the same efficiency: simulation of strain fields involving $\partial e_{zz}/\partial x$ and $\partial e_{zz}/\partial y$ strain gradient components would require enormous time.

Therefore we simplified the model suggested in [9–11] by excluding the $\partial e_{zz}/\partial x$ component (see Fig. 2). The strain field without the $\partial e_{zz}/\partial x$ gradient component can be expected at some distance away from the interface. A model of a silicon crystal in $\langle 230 \rangle$ orientation with the dimensions of $55 \times 55 \times 300$ nm^3 was built. Bending was applied in the X ($\langle 001 \rangle$) direction with the maximum shift of 0.03 nm at the mean thickness, which corresponded to $\sim 0.015^\circ$ maximum distortion at the entrance and exit surfaces.

CBED patterns were simulated for 200 kV accelerating voltage and 20 mrad convergence angle. Figure 3 shows simulated central CBED disks for the undisturbed (a) and bended (b) crystals, the experimental image (c) is represented for comparison. It is seen that the model describes semi-quantitatively different types of line splitting: in two and three components. Slight divergence in line positions should be attributed to the deviation of experimental high tension from the nominal 200 kV. We suppose that accounting for the $\partial e_{zz}/\partial x$ strain gradient component is necessary to explain the more complex splitting and broadening features, when further approaching the strained interface (see Fig. 1).

Thus we demonstrated by simulation the validity of the earlier suggested model for the explanation of HOLZ line splitting near the interface. Splitting occurs due to the bending of the crystal near the interface because of the strain relaxation in thin TEM lamella during sample preparation. Further we are going to quantify the effect. Quantification is necessary for the reconstruction of complete strain field in the TEM lamella, which in turn will allow the reconstruction of the strain state in the original bulk sample.

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