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Strain field reconstruction in shallow trench isolation structures by CBED and LACBED

A. Spessot [a,*], S. Frabboni [a], R. Balboni [b], A. Armigliato [b]

[a] National Research Center S3, CNR-INFM and Department of Physics, University of Modena e Reggio Emilia, Via G. Campi 213/A, 41100 Modena, Italy
[b] CNR-IMM Section of Bologna, Via P. Gobetti 101, 40129 Bologna, Italy

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Abstract

Using a combination of the CBED and the LACBED techniques in the transmission electron microscopy (TEM), we have investigated the strain field in the silicon active region of a shallow trench isolation structure, underlying a $TiSi_2$ layer. Starting from the analysis of the deformation in a sample, thinned for TEM analysis, we have reconstructed the displacement field, simulating the split HOLZ lines visible in the experimental CBED patterns. From the comparison between the experimental LACBED patterns, taken in a suitable sample orientation to evidence the stressors distribution in the polycrystalline silicide layer, and the corresponding dynamically simulated ones, we have reproduced the strain field in the unthinned, bulk sample.

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1. Introduction

In the last couple of decades it has been ascertained in the field of micro- and nano-electronics that one of the major issues in the current and future integrated circuit technologies is the mechanical stress built up in the layers and the silicon substrate [1].

When a stress source (stressor) is deposited on top of a thick crystalline substrate a strain field can be originated, deforming the original crystalline lattice. The stressor structure can be twofold: a *homogeneous* structure (such as a coherently deposited perfect single crystal) or a *microstructured* one (like a polycrystal). In both these cases, the only way to obtain strain measurements with a lateral resolution at the nanometer scale is the convergent beam electron diffraction of the transmission electron microscopy (CBED/TEM). This powerful technique is based on the analysis of the strain induced shift of high order Laue zone (HOLZ) deficiency lines, which occur in the central disk of a CBED pattern when the incident electron beam has a suitable convergence (typically of the order of 10 mrad) and is aligned parallel to a zone axis. A typical experimental CBED pattern, acquired from a perfect silicon crystal, is given in Fig. 1(a). The general procedure to obtain quantitative strain information from patterns like this, acquired in strained crystal, has been described elsewhere [2].

If strain gradients along the electron beam direction are negligible, a map of the strain can be obtained from the experimental CBED patterns in a semi-automatic way, without any assumption on the displacement field [3,4]. Otherwise, when strain gradients are present, the HOLZ lines are split in two components and intermediate fringes can be observed [5]: an example is given in Fig. 1(b).

By the use of a deformation model the split HOLZ line profiles can be reproduced, thus reconstructing the displacement field in a TEM sample with both a homogeneous [6] and a microstructured [7] stressor layer. To analyze the latter case, we have developed a new recursive method to fit the simulated 2D split HOLZ pattern to the experimental

* Corresponding author. Tel.: +39 059 205 5257; fax: +39 059 205 5235.
E-mail address: spessot@unimo.it (A. Spessot).

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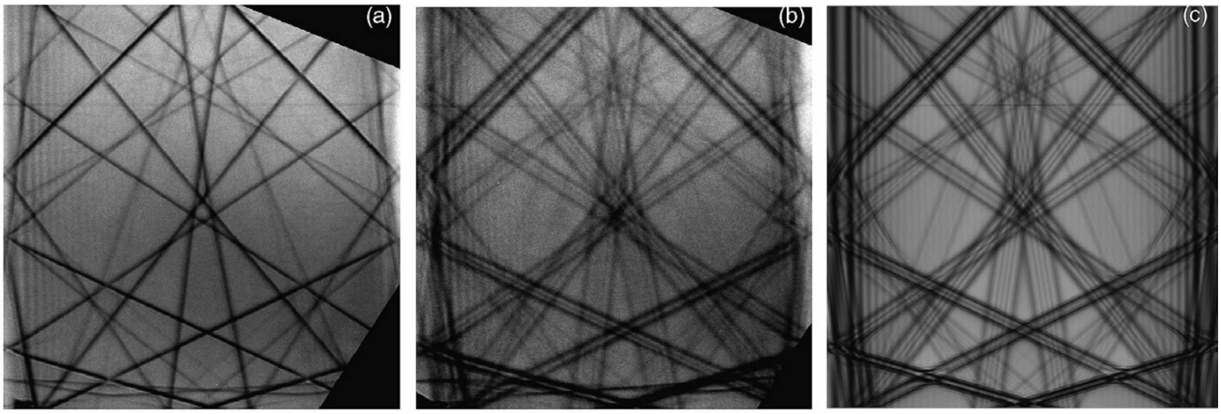

Fig. 1. (a) Silicon <230> TEM/CBED patterns taken at 200 keV in the undeformed substrate. (b) Pattern acquired in a deformed area of the sample in the same orientation and experimental conditions. A not negligible bending of the lattice planes along the electron beam direction is caused by the strain gradients, and the splitting of the HOLZ lines is clearly visible. (c) Corresponding dynamical simulation of the strained pattern in (b), assuming a radial displacement field.

ones, based on the refinement of a parametrized displacement model. This can be obtained by an analytical formulation or from finite elements analysis.

The CBED/TEM analysis requires thinning the bulk specimens to a typical thickness of hundreds of nanometers. It is well known that after thinning, the substrate and stressor can be arranged in a different configuration with respect to the bulk-like case. This can be caused by an inhomogeneous distribution of the strain source in the stressor layer deposited onto the thick specimen and/or in different elastic properties of the substrate and stressor. Therefore, the TEM results may not be directly representative of the bulk materials [8], and the original strain state must be reconstructed accounting for the relaxation of the free surface in the specimen after the thinning procedure.

For the single crystal structures, many authors perform this reconstruction both by different analytical approaches [9] or by finite element (FE) methods [10]. Otherwise, when the stressor layer is represented by a microstructured material, the reconstruction of the deformation in the thick specimen cannot disregard the local distribution of the stressor source in the layer.

In a previous work [7] we demonstrated that it is possible to reconstruct the displacement field in a thinned strained substrate underlying a structured stressor layer, thus accounting for the observed split HOLZ patterns. In this paper, we extend this method to map the strain distribution of a diagonal component of the strain tensor in a corresponding thick, bulk-like case of the same microstructured sample, by the combined use of the CBED and the large angle CBED (LACBED) techniques.

2. Experimental

The strain reconstruction has been performed in a sample where the deformations were induced by the formation of Ti–salicide overlayers onto the 0.18 μm wide active silicon areas of shallow trench isolation structures (STI). Additional details about the samples preparation and the experimental apparatus are given elsewhere [7].

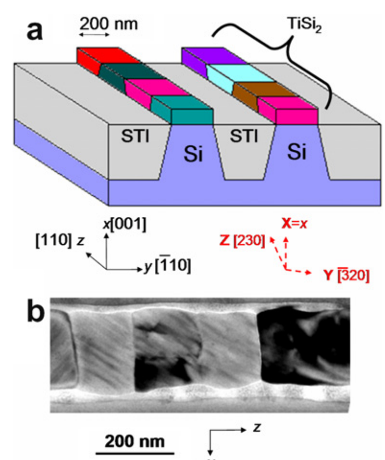

Fig. 2. (a) Sketch of the investigated structures. The $TiSi_2$ layer deposited on top of the silicon active region consists of a one-dimensional array of grain boundaries. (b) TEM plan view of the bamboo-like polycrystalline distribution in (a). The mean grain size in z direction is of the order of 100 nm.

As a result of the growing process of the $TiSi_2$ layer, a series of polycrystalline stripes of $TiSi_2$ is formed on top of the silicon active area; a sketch of the analyzed devices is given in Fig. 2(a). In Fig. 2(b) it is shown a plan view TEM micrograph taken in an area containing a salicide stripe. It is evident that the salicide consists of a so called bamboo-like [11] grain boundaries distribution in a one-dimensional array, that is a set of grains whose boundaries are almost parallel to each other and perpendicular to the axis of the stripe ([1 1 0] direction). Their thickness is about 100 nm, which is less than the typical local cross section thickness used for a CBED experiments (200–400 nm): thinning the specimen along the [1 1 0] direction, at least one grain boundary is included in the analyzed volume.