Phys. Status Solidi C **10**, No. 1, 28–31 (2013) / **DOI** 10.1002/pssc.201200548

physica status solidi pss c
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current topics in solid state physics

Dislocation formation during laser processing of silicon solar cell materials

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Received 31 July 2012, revised 28 August 2012, accepted 9 October 2012
Published online 11 December 2012

Keywords laser processing, dislocation formation, silicon solar cells, transmission electron microscopy

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Laser processing, increasingly used for solar cell production, induces defects when choosing inappropriate process parameters. Besides the shape and the pulse energy of the laser, also the surface orientation of silicon substrate has a great influence on the defect formation. By applying a laser beam with a line focus exceeding the critical values such as line width and laser pulse energy, the development of dislocations is observed on (111)-oriented wafers by transmission electron microscopy (TEM). As a result, the formed dislocations are arranged practically parallel to each other in planes parallel to the (111) surface. Their Burgers vectors lie within this plane too. Thus classical concepts of epitaxy hardly explain the dislocation formation. Alternative explanations have to take into account the excessively high temperature close to the melting point, the short time frames given by the laser pulse duration (100 ns) and the not yet analyzed inhomogeneous stress distribution.

1 Introduction Laser processing has emerged as one of the key technologies in today's solar cell industry to produce solar cells at reduced costs with systematically increased efficiencies η. Laser doping is easily incorporated in a solar cell fabrication sequence as it is considered an inline-process and thus reduces manufacturing costs. Also this technology is already widely applied to produce selective emitters after furnace doping [1]. A full area p-n junction produced this way leads to an efficiency of 18.9% [2], an additional absolute gain in efficiency of $\Delta\eta$ = 0.5% [1] was achieved in a selective emitter. Nevertheless, if the process parameters during laser doping are not properly chosen, the irradiation of the semiconductor can cause undesirable lattice defects to form. Furthermore, the fundamental understanding of the melting and recrystallization processes during laser doping is still fairly vague.

Depending on the process parameters, such as the crystal orientation of the silicon wafers, the shape and energy density of the laser pulse, mainly two types of defects are observed in our experiments. The (100)-oriented wafers that are irradiated by a circular laser focus with an overcritical pulse energy density show the formation of micro-cracks [3]. By using a laser beam with a line focus exceeding critical values of the line width and laser pulse energy, the development of dislocations has been observed on (111)-oriented wafers, but not on (100)-oriented ones [3]. The formation processes of both micro-cracks and dislocations are not known so far in detail, however, understanding of these is very desirable for the optimization of laser processing.

The present contribution focuses on the analysis of the formed dislocations and to arrive at first ideas of the formation process. In order to limit the influential parameters we consider laser crystallized pure (111) silicon substrates. By using transmission electron microscopy (TEM) in conjunction with large-angle convergent-beam electron diffraction (LACBED), details of dislocation arrangement and the Burgers vector population are analyzed. Dislocation arrangement and Burgers vectors exhibit at first sight the elements of epitaxial overgrowth, however, do not correspond to the well-known type of 60°-

dislocation misfit network that originates from glide processes, e.g. [4].

2 Experimental procedure In our experiments (111)-oriented p-type Czochralski wafers were irradiated by a pulsed Nd:YAG-laser operating at a wavelength of $\lambda = 532$ nm. The laser pulse had a duration of $\tau = 100$ ns. The width of line focus w varied in the range from 5 µm to 16 µm at full-width at half-maximum (FWHM), while the line length was fixed at 2.5 mm. The pulse energy density E_P was adjusted to fixed values between 0.7 J/cm^2 to 3.9 J/cm^2. For a full area laser doping, the laser beam is scanned over the wafer surface with overlaps, locally melting the silicon. After irradiation, on cooling, the silicon melt crystallized epitaxially. Hereby the scanning direction was along the short axis of the line focus, which was also along the direction of the primary flat indicating {110}-planes (in the (111)-oriented wafers: along the crystal orientation <112>). For details of the irradiation setups and procedures see Ref. [3].

The TEM observations of both plane-view and cross-section samples were carried out in a Philips CM 200 operated at 200 kV. The fine structures of dislocations were imaged using weak-beam dark-field (WBDF) technique. In order to determine the Burgers vectors, LACBED was used in combination with Cherns and Preston's evaluation rules [5]. A great advantage of LACBED-pattern is that it contains diffraction and image coevally, the evaluation is based on the number of splittings of Bragg lines at crossings with dislocation lines. The splitting number is directly related to the Burgers vector by the dot product with the indices of the Bragg lines.

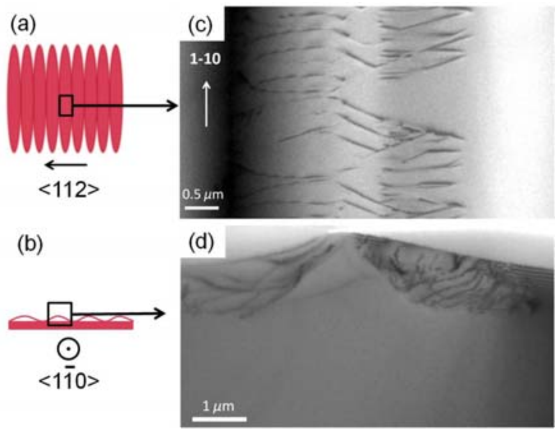

Figure 1 Illustrations of the irradiated area of a (111)-oriented wafer from the top (a) and from the flat (b) and the appropriate plan-view (c) and cross-section TEM bright field (d) images. After laser irradiation the surface shows a waved structure (b) at the flanks of which dislocation arrays have arisen (d, in multi-beam condition). The dislocations exhibit a quasi-periodic arrangement, which lie substantially parallel to each other and over long distances almost parallel to the (averaged) surface (c, **g** = < 2-20>).

3 Results and discussions On (111)-oriented wafers that are irradiated by a line focus having a width $w > 15$ µm and a pulse energy density $E_P > 3.7$ J/cm^2, dislocation development is observed. Figures 1a and 1b illustrate the irradiated area as seen from both the top and the flat of a (111)-oriented wafer.

The view onto the flat in Fig. 1b exhibits a wavy surface after irradiation. Dislocation arrays are observed in the flanks of each of these wave peaks in the cross-section TEM image (cf. Fig. 1d). The plane view in Fig. 1c shows these dislocations to be arranged in a characteristic quasi-periodic configuration almost parallel to the surface. This geometry suggests that they compensate a strain component mainly in the direction of the longitudinal axis of the irradiated area. The determined Burgers vectors (see below) will substantiate this assignment. The entangled structures between the dislocation segments are exemplified in Fig. 2. These interaction regions (cf. Fig. 2a) line up in the direction of the long axis of the laser focus. At higher magnification (cf. Fig 2b) the fine structure consists of a complicated dislocation network including stacking faults and three dimensional dislocation interactions.

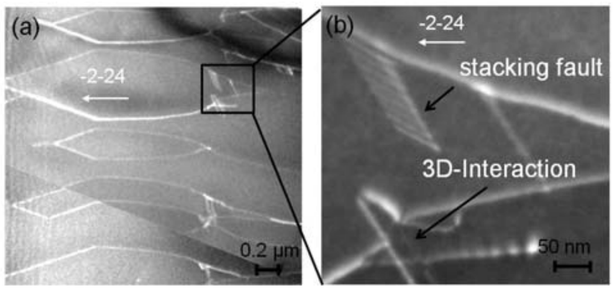

Figure 2 Fine structure of the dislocation arrangement in (111)-oriented wafers. Plan-view micrographs in weak beam. (a) The bright dislocation lines lie parallel to each other in two respective directions. (b) Magnified view of the entangled structure with stacking faults and dislocation interactions.

The Burgers vectors of the dislocations are determined by applying the Cherns and Preston's approach to areas of dislocations like in Fig. 2a. The quasi-periodic arrangement of dislocations aids the Burgers vector determination of an appreciable number of dislocations from one micrograph only. Figure 3 shows an example of an evaluation where the colors of the drawn dislocation lines represent the corresponding Burgers vectors. These colors are identified in terms of Burgers vector type in the Thomson tetrahedron that depicts all perfect (solid lines) and partial Burgers vectors (dashed lines) contained in the (111) plane of the wafer surface. The Shockley partial dislocations with the Burgers vectors $a/6[2\text{-}1\text{-}1]$ and $a/6[\text{-}12\text{-}1]$ and the associated perfect edge dislocation with a Burgers vector $a/2[1\text{-}10]$ (along the long axis of the irradiation area) dominate (cf. Fig. 3). The black colored curves indicate the dislocations having a Burgers vector *a*/2[011]. The grey dotted segments mark the dislocations that cannot be identified from the given geometry and selected LACBED-pattern. As a result most of the Burgers vectors lie in the (111)-plane parallel to the surface. This observation is at variance with other work [4], which found dislocations having their Burgers vectors obliquely to the surface plane. Matthews et al. (cf. Ref. [6]) showed that such dislocation networks can relax the two-dimensional stress state of a heteroepitaxial layer.

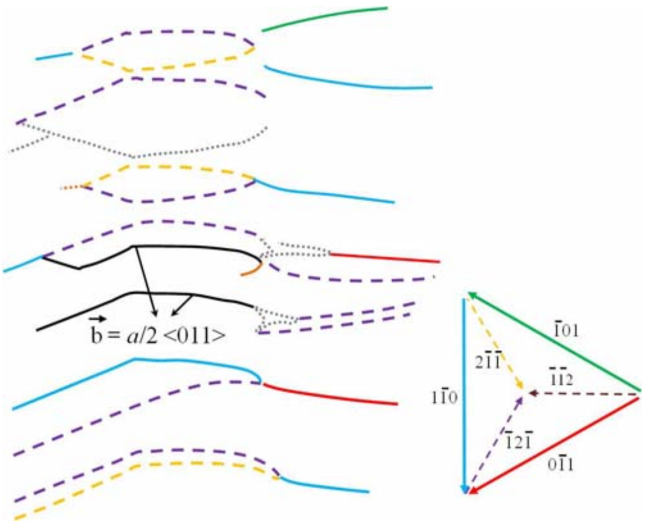

Figure 3 Dislocations are illustrated in different colors combining with three types of lines (solid, dashed and dotted) due to different Burgers vectors. The Burgers vectors are color coded with the aid of the introduced vector sketch of the (111) plane parallel to the wafer surface. The solid curves indicate the perfect dislocations, while the dashed ones mark the Shockley partial dislocations. The dotted curves denote the dislocations that cannot be identified in the selected LACBED-pattern.

In order to explain our observed dislocation arrangement, one can start from this idea of stress relaxation. We may describe the situation as heteroepitaxy where a hot (compressively stressed) silicon layer is epitaxially situated on a cold substrate giving rise to a plane stress state. In fact the sum Burgers vector of the observed dislocations is essentially along the long axis of the laser spot and thus will compensate a corresponding stress component in this direction (the dislocations act as effective edge dislocations). However, one runs into difficulties when describing in this notion the dislocation formation process. When we consider glide, then the dislocations need to have Burgers vectors that lie obliquely to the surface plane which is not the case. Climb can be ruled out since such dislocations need to have pure edge character and also generally have a rather irregular course of their lines on rather small scale due to locally fluctuating incorporation of atomic defects. In our case both conditions are not fulfilled. Thus an alternative explanation is required. Possible explanations could be based on the wavy surface that relaxes the condition of a planar stress field. Then shear stress can arise in the surface-parallel glide plane. Another possibility is suggested by the observation of the dense tangles just below the crests of the wavy surface. These may act as local stress centers (without relaxing the condition of an over-all planar stress field) causing the required shear stress within the surface parallel glide planes. Such clusters can lead to some type of pencil glide (glide of a prismatic dislocation loop perpendicular to its plane, e.g. [7]). The unknown level, distribution and temporal development of the stress field prevent a further analysis presently. One has to keep in mind, that with laser processing we have entered the field of dislocation processes at very high temperature (up to melting point Si) at a rather short time period (e.g. laser pulse duration 100 ns) about which knowledge is still very limited aggravated by an undetermined inhomogeneous stress distribution.

4 Summary

We have investigated by using transmission electron microscopy the dislocation network that is formed during laser processing of (111)-oriented silicon wafers under certain process parameters. The formed dislocations arrange essentially parallel to the wafer surface as a set of practically parallel dislocation lines that all run perpendicular to the long diameter of the elliptical laser spot. As an important result the Burgers vectors predominantly lie in the (111) plane which is parallel to the surface. This result could fit into the common dislocation relaxation pattern of an expanded silicon layer epitaxially confined to a cold silicon substrate. However, the partial and perfect Burgers vectors lying within a surface parallel glide plane do not. Dislocations of this type cannot reach such positions by glide. However, glide has been analyzed under experimentally different conditions (comparably slow cooling), e.g. [4]. In principle the dislocations in our samples could assume their positions by climb [8], however, would assume rather irregular line shapes in contrast to our observation. Nevertheless, they point to the important task, to first identify the stress distribution and its time development in the short time frame imposed by the laser pulse duration of 100 ns and to extend the defect behavior to this high temperature-short time parameter field.

Acknowledgements The authors would like to thank the members of Stuttgart Center for Electron Microscopy (StEM) for the great support in TEM measurements. M. Kelsch and M. Strafela were of indispensable help in sample preparation. A special thank you goes to F. Benz for his valuable comments and fruitful discussions.

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