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A particular case of electronic behaviour of the $\Sigma = 3$ grain boundary in p-type Si

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Abstract. Electrical conductivity measurements combined with transmission electron microscopy observations were performed on a p-type Si bicrystal containing a $\Sigma = 3$ coincidence site lattice grain boundary. An increased conductivity observed in the surroundings of the grain boundary is due to the formation of a potential well for the holes. The potential well is found to be due to the segregation of impurity atoms, which saturate existing free bonds in the core of the observed dislocations at the interface.

1. Introduction

During the last two decades the interest in polycrystalline Si, which is used in microelectronics [1] and solar cells applications [2], has been focused on the study of grain boundaries (GBs). A representative review paper of this field has been presented by Grovenor [3]. The interesting electrical properties of poly-Si are attributed to the presence of GBs, but the final result depends on the structure of the GBs and their interaction with the electrical charge carriers. Most of these interfaces are coherent twins or twin-related boundaries and therefore they are electrically inactive in as-grown crystals [4]. On the other hand, the electrical activity of as-grown GBs is correlated, in some cases, with the dislocation density in the boundary plane [5]. Dislocations and facets reduce the electrical properties of GBs and this behaviour is associated with segregated atoms [6].

A typical GB frequently observed in polycrystalline Si is the coherent $\{111\}$ twin described, by means of the coincidence site lattice (CSL) model, as a $\Sigma = 3$ CSL. This GB has been characterized as electrically inactive [7–9].

The aim of this work is to present the peculiar electrical behaviour observed in a $\Sigma = 3$ CSL GB of an as-grown Si bicrystal. The results are based on electrical conductivity measurements as well as on transmission electron microscopy (TEM) studies. Thus, a connection between the electronic behaviour and the observed structural defects in the boundary plane is achieved.

2. Experiment and results

2.1. Electrical measurements

For the electrical conductivity measurements a circular flat sample in the form of a twin bicrystal was cut from a polycrystalline silicon ingot grown by the Bridgman method. The diameter of the sample was 14.90 mm and its thickness 0.267 mm.

The sample which contains the twin, together with the shape, the position, the direction and the dimensions of the contacts used for the electrical measurements is presented in figure 1. Six Al strips (A to F) were evaporated on the upper surface of the sample, parallel to the interface, i.e. three strips on each side of the boundary. With this contact arrangement it was possible to measure the resistivity of the two crystalline parts of the sample and also of the area including the grain boundary by a four-point method. The Al electrodes were evaporated under vacuum and then the sample was heated at 400 °C under vacuum (10^{-4} mm Hg) for several hours. Following this procedure, ohmic contacts of low resistivity were formed with the Si bicrystal. The contact properties were subsequently tested by a four-point method, using the two outer electrodes to provide the sample with the current and by measuring the voltages between the four inner contacts. In the range 1 μV to 10 mV, the ohmic behaviour was tested. All measurements reported were done in this ohmic region. A final test, by means of test, by means of thermal EMF investigation, showed that both grains of the bicrystal were p-type.

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