Crystallographic defects in orthorhombic ScSi / Si(001) contacts

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1. Introduction

Orthorhombic ScSi (COD card no. 00-000-9969, mp-9969, [1]) has been identified in the top part of lowly resistive TiN / ScSi / ScSiP / Si:P / Si(001) contact stacks showing great potential for NMOS devices [2-3]. However, little is known about its precise formation mechanism and contribution within the stack. In a previous publication [4], the analysis of X-ray diffraction (XRD) pole figures revealed that orthorhombic ScSi / Si(001), formed via solid state reaction, has an epitaxial texture with two different components having a (010) and (130) out-of-plane orientation (referred to as 'epi 1' and 'epi 2' in the following). Both components have a ScSi(002) // Si(220) in-plane alignment. Additionally, the epi 1 grains are aligned in-plane along a second independent direction: ScSi(200) // Si(220). Despite having identified these two orientations, the nanostructure and interface properties of the corresponding grains are not known. This work aims at bridging this gap by correlating the macro scale structural properties with local nano-structural inspections by cross section transmission electron microscopy (XTEM).

2. Methods

The sample consists of 10 nm TiN / 17 nm ScSi / Si(001) obtained by solid state reaction between a nominally 15 nm thick Sc thin film and a Si(001) substrate. Physical vapour deposition (PVD) is used to deposit the Sc and TiN layers. These layers are deposited without vacuum break. Prior to deposition, a wet etch in diluted HF is performed to remove the native oxide. TiN acts as a capping layer to prevent oxidation of the underlying ScSi. Following deposition, the sample is annealed in forming gas (10% H_2 in N_2) at 420°C for 20 min, resulting in the formation of orthorhombic ScSi [3]. Nano-structural inspections are carried out using XTEM. All XTEM images are taken along the Si<110> zone axis. Complementary energy dispersive X-ray spectroscopy (EDS) analysis confirms the formation of ScSi monosilicide (not shown).

3. Nano-structural analysis of orthorhombic ScSi / Si(001)

Figure 1(a) shows a large-scale bright-field transmission electron microscopy (BF-TEM) cross-section image of the stack. The Si substrate, ScSi layer and TiN layer can be clearly distinguished and are labelled for clarity. The ScSi layer is polycrystalline. Two distinct regions can be observed: region 1, containing small ($\lesssim$ 5 nm) nano-twinned grains and region 2, containing large ($\gtrsim$ 20 nm) grains that are horizontally and vertically aligned with the substrate. The orientation of the ScSi grains in these two regions is further investigated in Fig. 1 (b) – (d). Figure 1(b) shows multiple nano-twinned grains. As a result of the small size of the individual grains, a strong streaking effect can be observed in the fast Fourier transform (FFT). In between the nano-twinned regions, some larger grains can be observed (Fig. 1(c)). These grains correspond to the epi 1 texture component. Comparing Fig. 1(b) and Fig. 1(c) evidences that the nano-twinned grains correspond to epi 1 ScSi and epi 2 ScSi with their twin boundary along the (110) plane of the epi 1 grain. Indeed, the mirror image of epi 1 ScSi across the (110) plane (equivalent to a rotation of 42° about its c-axis) results in the epi 2 orientation as found in [4]. The ScSi grain shown in Fig. 1(d) also corresponds to epi 1. However, its in-plane component is rotated 90° about the b-axis compared to Fig. 1(c).

4. Crystalline defects in orthorhombic ScSi / Si(001)

The analysis outlined in the previous section reveals that the growth of ScSi along its a-axis (region 1) is associated with the formation of {110} twin defects that propagate through the full ScSi layer, resulting in a small grain size ($\lesssim$ 5 nm). The epi 2 ScSi grains are only present in this region and are twinned versions of the epi 1 ScSi. This agrees with the low peak intensity observed in XRD for the epi 2 orientation [4]. The small grain size and large defect density (roughly 1 twin defect every 1 – 5 nm) may be detrimental to the contact performance.

Finally, the growth of ScSi along its c-axis is further investigated. Figure 1(e) shows a HRTEM of the ScSi / Si interface for a ScSi grain oriented in the same way as in Fig. 1(d). The corresponding FFT image shown in Fig. 1(f) reveals the lattice mismatch between ScSi{002} and Si{220}. The alignment between these planes is visualized in the ScSi{002} / Si{220}-filtered inverse FFT shown in Fig. 1(g). The planes are epitaxially aligned across the contact interface. However, there is a misfit dislocation at the ScSi / Si interface every ~ 23rd plane. This domain-matching epitaxy [5] is expected given the large mismatch between the ScSi{002} and Si{220} interplanar spacings (Δd = 0.086 Å). Additional FFT analyses reveal that the remainder of the ScSi in this region is nearly defect free (not shown).

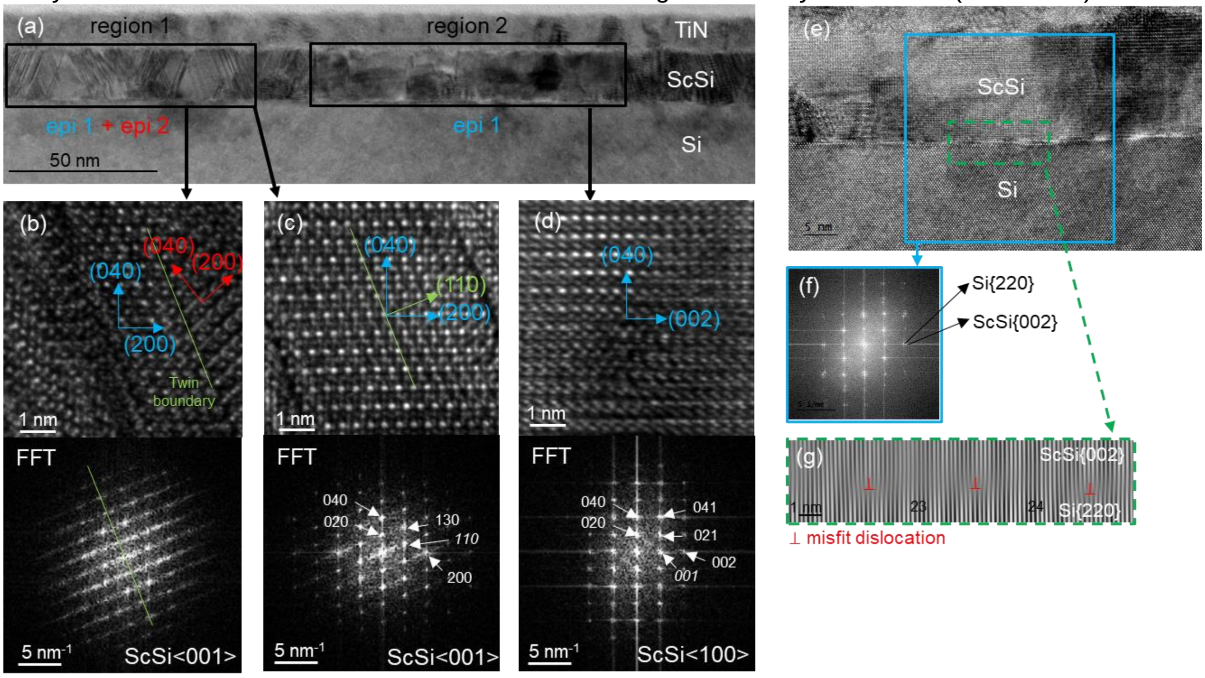

Fig. 1: (a) Large-scale BF-TEM image of a 10 nm TiN / 17 nm ScSi / Si(001) contact stack. HR-TEM images and corresponding FFTs taken in region 1 ((b) – (c)) and in region 2 (d). The FFT patterns are indexed using orthorhombic ScSi oriented along the indicated zone axis. The FFT spots indexed in italic correspond to kinematical forbidden diffraction spots. (e) HRTEM image of ScSi / Si(001), oriented according to Fig. 1(d). (f) FFT image extracted from the ScSi / Si(001) interface. (g) Corresponding ScSi{002} / Si{220} FFT filtered image.

5. Conclusions

The nanostructure and defectivity of orthorhombic ScSi / Si(001) contacts are investigated by XTEM. The analysis reveals that the growth and resulting nanostructure of ScSi is strongly anisotropic. The growth along ScSi<001> // Si<110> results in domain matched epitaxy, having a minimal defectivity limited to 1 misfit dislocation located at the contact interface every ~ 4.4 nm. The growth along ScSi<100> // Si<110> on the other hand, results in a higher density (up to ~ 1 defect / nm) of ScSi{110} twin defects, which propagate through the full ScSi layer. The former growth mechanism is expected to be preferred for optimal contact performance. Hence, it is hypothesized that a further improvement in contact resistivity could be achieved by controlling these growth mechanisms, and hence extend epi 1 grains along ScSi<100>, during the formation of orthorhombic ScSi. The origin of the growth anisotropy will be investigated as a first step to enable this.

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