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Interface and Structural Characterization of Buried $CoSi_2$/Si(001) Nanoplatelets

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There has been great interest in metal silicides investigation due to the potential applications as contact materials in microelectronic devices (e.g. TiS_2, CoS_2, NiS_2) [1]. These materials have been extensively studied on the past two decades with particular notability for the cobalt disilicide. $CoSi_2$ is a low electrical resistance material with CaF_2-like structure (*Fm3m*), which is similar to the diamond-like structure of Si (*Fd3m*). The relatively small lattice mismatch of nearly 1.23% between $CoSi_2$ and Si and the structural similarity leads to the possibility of growing epitaxial thin films and buried nanostructures along the (001) or (111) planes [2]. The knowledge of the crystal shape and of the $CoSi_2$/Si interface is essential for the theoretical modeling of these systems because these features have important influence on the electronic behavior, in particular the Schottky barrier height. Here is presented a comprehensive high resolution transmission electron microscopy (HRTEM) investigation of buried $CoSi_2$/Si nanostructures unconventionally obtained from a soft-chemistry method. In addition, the HRTEM images were studied by a strain state analysis method (GPA) [3] to calculate the 2D lattice distortion around the nanostructures. These results were compared with predictions as obtained by Finite Element Simulation (FE) to verify the induced 3D strain state.

The samples were prepared using a sol-gel method by hydrolyzing TEOS with cobalt nitrate. The solution was spin-coated on Si(001) substrates followed by heat treatment for calcination and reduction in an H_2-Ar environment. Cross-section TEM specimens were prepared along the Si[110] zone axis by mechanical polishing and gentle ion milling. A JEM-2100 HTP with LaB_6 electron gun was used at 200 kV. Exit-wave focal series reconstruction was used to obtain phase images with improved spatial resolution and atomic columns positions. The geometric phase analysis method was used to calculate the 2D strain/stress state from HRTEM images. The FE investigation was performed from commercial FE software with anisotropic elastic properties by setting an initial strain condition due to the local lattice mismatch between the strained nanostructure and the substrate.

Figure 1.A shows a typical low magnification TEM image with three $CoSi_2$ buried nanostructures (which were formed by Co diffusion from the silica film to the Si substrate), where a careful analysis by sample tilting reveals a hexagonal nanoplatelet shape (Figures 1.B-E). These nanostructures grow on the {111} silicon plane family (habit plane) with a highly uniform shape and thickness (3.2 nm). Figures 2.A and 2.B show a representative HRTEM image of a typical nanoplatelet and the exit-wave reconstructed phase image, respectively. These images indicate the occurrence of a 8A interface [4], where the silicide interface is formed by an 8-fold coordination with the same orientation as Si(111). In addition, the images show the existence of two evenly spaced planar defects along the platelets. The strain state analysis methods suggests the occurrence of a strain relaxation process as induced by these defect formation.

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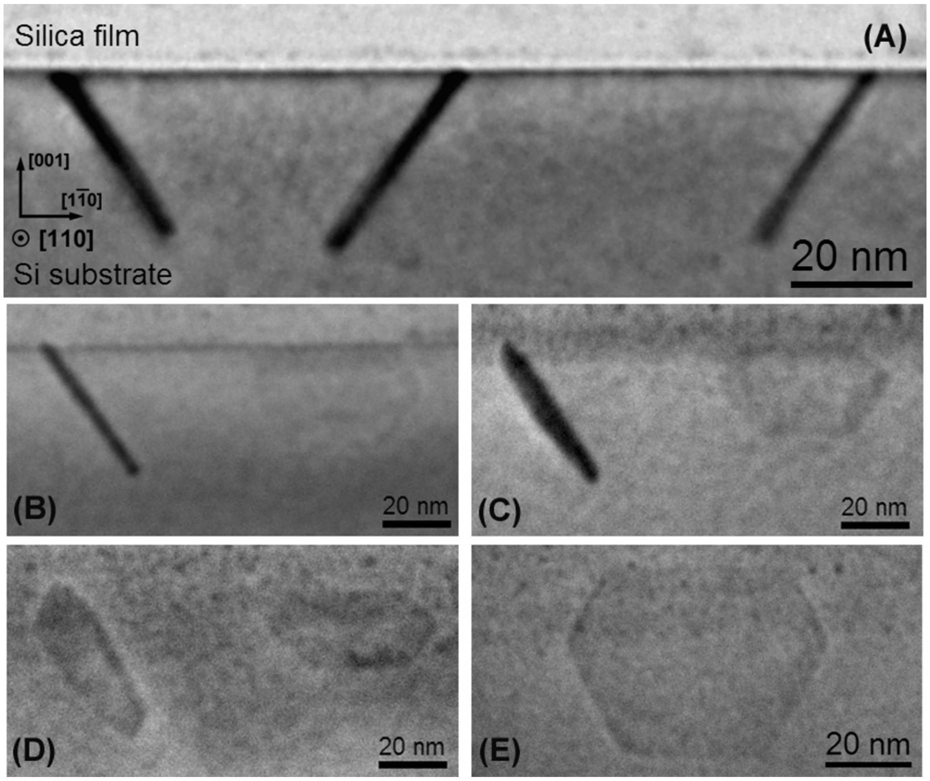

FIG. 1. (A) Low magnification TEM image of representative buried $CoSi_2$/Si(001) hexagonal nanopletelets along the Si[110] zone axis, where the Si substrate and the silica film are indicated. (B-D) TEM images of hexagonal nanoplatelets with sample tilting of 0, 15 and 30 degrees, respectively. (E) Typical TEM image of a hexagonal nanoplatelet front view.

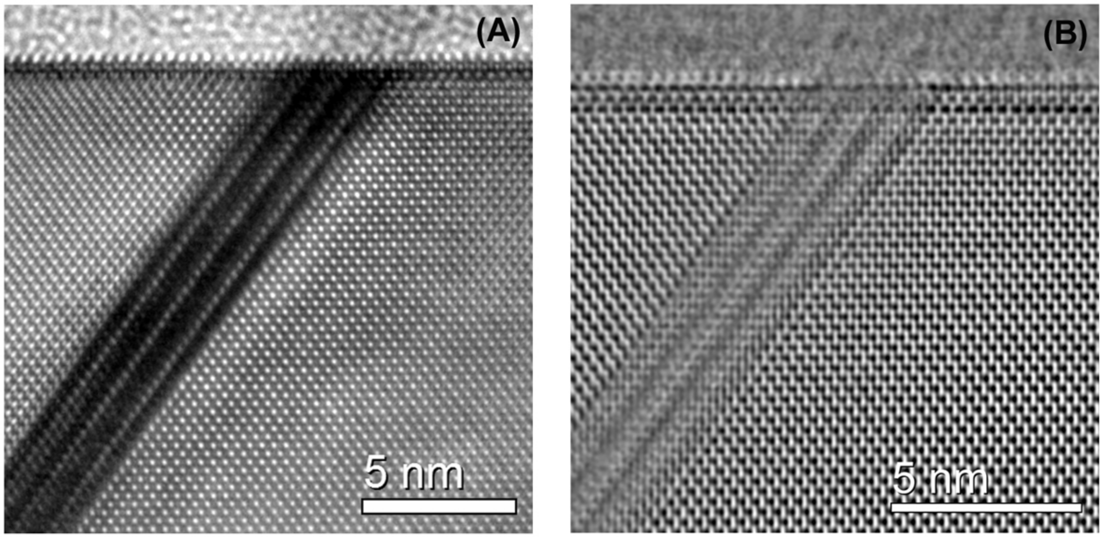

FIG. 2. Cross-section of $CoSi_2$/Si(001) typical hexagonal nanopletelets along the Si[110] zone axis (A) HRTEM image of a typical hexagonal nanoplatelet. (B) exit-wave reconstructed phase image, obtained by using focal series restoration.