

## 3-D analysis of semiconductor dopant distributions in a patterned structure using LEAP

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### Abstract

This work presents the first 3-D analysis of lateral dopant diffusion in a patterned structure using a pulsed laser-assisted local electrode atom probe (LEAP). A structure similar to a device channel was created for this work by performing a 3 keV,  $1 \times 10^{15} \text{ cm}^{-2} \text{ As}^+$  implant on a poly-Si line patterned wafer with 70 nm line width and 200 nm line pitch. The wafer was subsequently annealed at 950 °C for 1 s. LEAP samples were made using a site-selective in-situ focused ion beam (FIB) process. The results from LEAP analysis were then compared with high-resolution transmission electron microscopy (HRTEM) and Florida object-oriented process simulator (FLOOPS) results. Good structural agreement was found between the LEAP and HRTEM results. Several 1-D As concentration profiles extracted from the LEAP data were also found to be in good agreement with FLOOPS process simulation results. These profiles also represent for the first time that results from a 3-D process simulator have been able to be confirmed experimentally using a single sample.

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**Keywords:** Local electrode atom probe; Dopant characterization

### 1. Introduction

The channel length of a transistor has a critical impact on the device's performance. If significant lateral dopant diffusion occurs during post-implantation device processing, short channel effects can rapidly degrade device performance. To fully characterize lateral diffusion, dopant location must be measured along the entire length, width, and depth of the channel. Quantitative measurement of dopant location in 3-D, however, has proven challenging and most existing compositional analysis techniques than average measurements over one or two dimensions. Instead, channel widths are typically predicted using simulations and indirectly calculated from electrical measurements of completed devices. Thus, interest in atom probe tomography (APT) as a compositional analysis technique to measure lateral diffusion in semiconductor device structures has increased due to its ability to generate 3-D atomic maps of a sample.

Conventional geometry APT using pulsed-voltage field evaporation is most easily able to produce 3-D atomic maps of needle-shaped metallic specimens. Through the use of laser-assisted field evaporation, analysis of semiconducting materials has also been shown to be possible with conventional geometry atom probes (APs) [1]. These tools, however, have been limited by a relatively narrow ( $\sim 50$  nm) field of view and slow data collection rates (pulse repetition rate of 1–2 kHz) [2]. More recently, the development of the local electrode atom probe (LEAP) has increased the field of view to  $\sim 100$  nm and pulse repetition rate to 100 kHz while maintaining the 750:1 FWHM mass-to-charge resolution of reflectron-based APs by locating a local electrode near the sample tip [2]. Laser-assisted field evaporation may also be used with the LEAP to allow the analysis of semiconducting materials. Thus, it has been expected by the ITRS that APT, and more specifically LEAP, will be able to provide the metrology needed to fully characterize lateral dopant diffusion into the channel region of a device [3]. This work presents the first 3-D atomic scale analysis of a simple device structure using LEAP and compares the results to high-resolution

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transmission electron microscopy (HRTEM) and Florida object-oriented process simulator (FLOOPS) results.

## 2. Experiment

A patterned structure representing a transistor channel and gate was created on a  $\langle 100 \rangle$  Si wafer. First, 50 nm of poly-Si was deposited on top of a 1.5 nm thermal oxide. The wafer was then patterned and dry etched to produce parallel poly-Si lines of 70 nm width and 200 nm pitch. These lines, and the oxide beneath them, represent gate structures. The wafer was then implanted with 3 keV,  $1 \times 10^{15} \text{ cm}^{-2} \text{ As}^+$ . The poly-Si lines acted as a mask to create implanted regions, analogous to source/drain extensions, between each line. Once implanted, the wafer was spike annealed at 950 °C for 1 s to induce As diffusion.

LEAP samples were prepared from the wafer using an FEI DB235 focused ion beam (FIB). To protect the device structure from Ga damage during FIB processing, the wafer surface was coated with 200 nm of poly-Si. A site-selective in-situ liftout technique similar to that performed by Miller et al. [4] and Thompson et al. [5] was then used to prepare AP tips from the patterned region of the wafer. First, a 200 nm in-situ Pt deposition was performed directly over a channel feature to provide additional protection during FIB processing. A wedge containing the channel area was then cut from the surrounding bulk. Next, the wedge was attached to an Omniprobe in-situ micromanipulator using an in-situ Pt deposition, lifted free of the bulk, and positioned on top of a 100  $\mu\text{m}$  tall Si post created via a deep reactive ion etch (DRIE) process. The wedge was then attached to the Si post with another in-situ Pt deposition and cut free from the micromanipulator. Fig. 1A shows a scanning electron microscopy (SEM) image of the mounted wedge containing (1) the protective poly-Si coating, (2) the structure of interest, (3) Si substrate, and (4) Pt deposition attaching the wedge to the post.

Once mounted, the sample was FIB sharpened into an AP tip using a series of annular milling patterns. A SEM image of the final AP tip is shown in Fig. 1B. Note that no in-situ deposited Pt remains in the final sample tip and that the poly-Si line pattern is clearly evident in the images.

The AP samples were then analyzed using an Imago LEAP 3000X equipped with pulsed laser-assisted field evaporation. The sample was analyzed with UHV background pressure at a cryogenic base temperature between 20 and 100 K. A voltage between 3 and 10 kV was applied to the tip and field evaporation was induced by a green laser with sub-nanosecond pulse duration and spot size less than 10  $\mu\text{m}$  FWHM. Evaporation rate for the sample was greater than 0.02 ions/pulse. Over 20 million ions per sample were collected. 3-D atomic maps were then reconstructed from the LEAP using Imago Interactive Visualization and Analysis Software (IVAS). For comparison to LEAP results, HRTEM was performed on the experimental structure. The cross-section sample, oriented perpendicular to the line pattern, was FIB milled from an area adjacent to the location used to make LEAP samples. The TEM sample was imaged in bright field along the  $\langle 110 \rangle$  zone axis using a JEOL 2010F HRTEM. For additional comparison, the 3-D process simulator FLOOPS [6] was also used to simulate the implant and diffusion processes in the experimental structure. Accurate structural geometry with a slight recess outside the gate edge was input into FLOOPS. The diffusion models in the simulation included the effects of implant damage and concentration-dependent As diffusion using a set of consistent models [7]. In addition, a description of the temperature–time profile of the 1 s spike anneal was explicitly used for the thermal cycle.

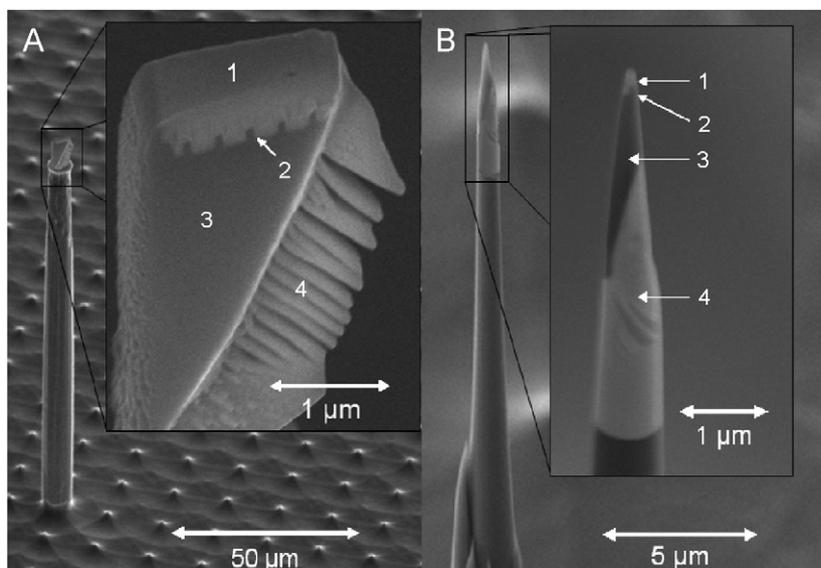


Fig. 1. SEM images of (A) mounted wedge containing (1) the protective poly-Si coating, (2) the structure of interest, (3) Si substrate, and (4) Pt deposition attaching the wedge to the post. (B) AP tip FIB milled from the wedge with areas indicated as in (A). Both SEM images were taken at 52° from vertical.

### 3. Results and discussion

Fig. 2A presents a side view of a portion of a LEAP-generated 3-D atomic map of the experimental structure. Of the 20 million atoms collected, only 10% of the O, 10% of the As and 0.1% of the Si atoms are shown for clarity. This is the first 3-D atomic-scale image of dopant and impurity atoms within a model Si device structure ever obtained. An HRTEM image of an identical structure is shown in Fig. 1B for comparison. The presence of the wafer's thermal oxide layer between the poly-Si pattern and the bulk, analogous to a gate oxide, can be seen in both images. It is also evident in both images that a thin oxide layer had formed on the poly-Si patterned lines. Finally, both images show a rough surface where implantation has occurred. This roughness is likely a result of the etching during patterning combined with defects generated during the amorphizing As<sup>+</sup> implantation and the regrowth of the amorphized region during the spike anneal. It is important to note that when viewing the 3-D atom map from the side as in Fig. 2A, the roughness causes the As implant, oxide layer, and poly-Si interface to appear qualitatively less abrupt than it is. Fig. 2C shows the 2-D FLOOPS process simulation results of the implant and diffusion processes. Isoconcentration contours are plotted for As concentrations between  $1 \times 10^{17}$  and  $1 \times 10^{21}$  atoms/cm<sup>3</sup>.

Several 1-D As composition profiles were extracted from both the LEAP and FLOOPS data for comparison. To generate the 1-D profiles, identical regions were selected in both data sets and subdivided into a series of smaller volumes. The average As composition in each subvolume was then determined. Error bars for the LEAP data were calculated treating each subvolume as a Bernoulli sequence [8].

Fig. 3A presents a profile extracted from a vertical cylinder with 12 nm diameter, divided into 0.5 nm subvolumes, located in the As implanted area, at least 8 nm from the gate edge. Approximately 3000 atoms are contained in each subvolume allowing LEAP compositional analysis, assuming a density of  $5 \times 10^{22}$  atoms/cm<sup>3</sup>,

to a concentration of  $1.66 \times 10^{19}$  atoms/cm<sup>3</sup>. The simulation and experimental results match well above this threshold with LEAP analysis giving a peak concentration of  $1.75 \times 10^{21}$  atoms/cm<sup>3</sup>, slightly higher than the FLOOPS peak concentration of  $1.45 \times 10^{21}$  atoms/cm<sup>3</sup>.

Lateral profiles were also extracted from the simulation and experimental results. For these profiles, rectangular regions measuring 2 nm vertically, 35 nm laterally, and 30 nm parallel to the line edge were subdivided laterally into 0.5 nm slices. For the LEAP data, a running average of four subvolumes was used to reduce the compositional variation induced by the small sample size of the subvolumes. Approximately 6000 atoms are contained in each averaged subvolume allowing LEAP compositional analysis to a concentration of  $8.33 \times 10^{18}$  atoms/cm<sup>3</sup>. Fig. 3A–C shows compositional profiles for rectangular regions centered at 3, 5, and 7 nm below the gate oxide. The approximate location of the line edge is indicated by a vertical dashed line. These profiles show good agreement to the simulation values though some local variation is present. A profile was not calculated within the first 2 nm below the oxide as the surface roughness seen in this region in both the LEAP and HRTEM data would cause excessive variability in the analysis.

### 4. Conclusions

This work shows that 3-D characterization of dopant distributions in a patterned semiconductor device structure is possible with the combination of pulsed laser-assisted field evaporation and local electrode geometry. Site-specific AP samples were shaped using an in-situ FIB process and analyzed with LEAP and HRTEM. Good comparison was found between the 3-D atomic map and TEM micrograph. Composition profiles extracted from the atomic map were also compared with FLOOPS process simulation results and found to agree well. These profiles represent the first time that results from a 3-D process simulator have been able to be confirmed experimentally. The ability to

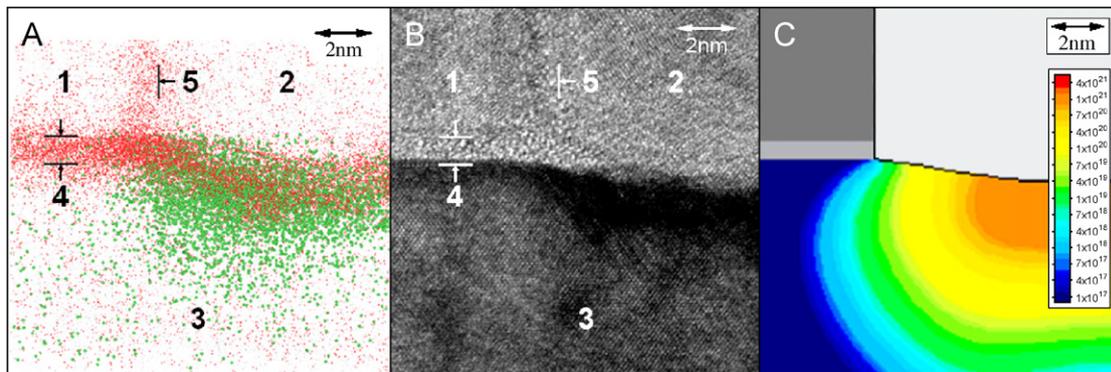


Fig. 2. (A) Side view of 3-D atom map showing (1) poly-Si patterned region (2) poly-Si coated region (3) Si substrate (4) SiO<sub>2</sub> thermal oxide and (5) poly-Si patterned line edge (red dots: oxygen atoms, green dots: arsenic atoms). (B) HRTEM image of an identical feature with areas indicated as in (A). (C) 2-D FLOOPS process simulation results with isoconcentration contours plotted for As concentrations between  $1 \times 10^{17}$  and  $1 \times 10^{21}$  atoms/cm<sup>3</sup>.

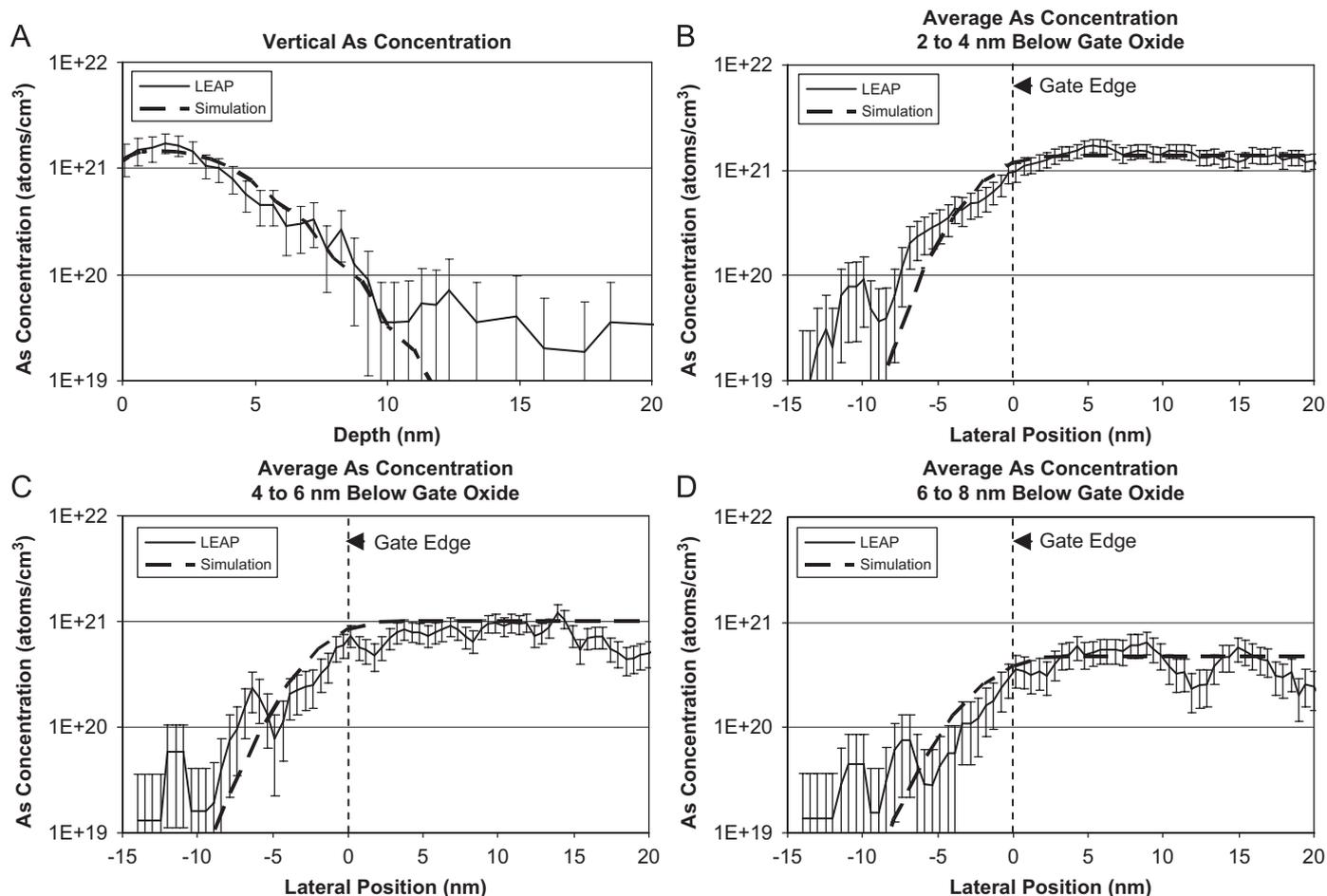


Fig. 3. 1-D As composition profiles extracted from LEAP and FLOOPS simulation data for (A) vertical cylinder 12 nm in diameter, subdivided into 0.5 nm vertical slices, located away from gate edge; (B) rectangular region of 2 nm  $\times$  30 nm  $\times$  35 nm, subdivided into 0.5 nm lateral slices, centered at 3 nm below the gate oxide; (C) identical rectangular region centered 5 nm below the oxide and (D) identical rectangular region centered 7 nm below the oxide.

experimentally verify simulation results will allow substantial improvements in device modeling and design.

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