Heating effects in Bi-doped Cu nanowires for spintronics: atomic resolution in-situ insights

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Background incl. aims
CuBi alloys are predicted to exhibit a giant spin Hall effect (SHE), making them promising materials for developing spintronic devices. This prediction was supported by the direct observation of SHE in Cu95Bi5 films by X-ray spectroscopy. However, the material composition and structure, e.g. crystallinity, crystallite size, effective Bi insertion into the Cu lattice or formation of metallic clusters of Bi, can affect the spin Hall angle, which is related to the efficiency of the spin-to-charge current conversion. This efficiency becomes more and more critical in the case of reduced dimensionality systems, where some dimensions may become smaller than the spin diffusion length. Changes taking place during device operation, such as those related to Joule heating, may also affect the system performance.

Methods
Here, we present a detailed structural characterization of Bi-doped Cu nanowires (NWs) with a high Bi doping level (up to 7% Bi) and different degrees of crystallinity, grown by template-assisted electrochemical deposition. The combination of in-situ atomic resolution scanning transmission electron microscopy (STEM), diffraction, electron energy-loss spectroscopy (EELS) and high-resolution synchrotron powder X-ray diffraction (PXRD), allows studying in detail the atomic structure of the NWs, which is critical for optimization of the spin transport related properties.

Results
Nanodiffraction (4DSTEM) measurements were used to analyze the crystallite size and orientation of the nanowires (see Figure 1(a,b)), allowing to harness the growth procedures in order to achieve a controlled distribution of grain boundaries, with average crystal sizes ranging from tens of nm to the micron scale. In-situ heating experiments, using both STEM and PXRD techniques, were carried out to reproduce operando conditions subject to Joule heating effects. After heating for an interval of several minutes at 400°C, in-situ PXRD measurements show that a temperature induced structural transition takes place. For an initial Bi doping of 6%, diffraction peaks typical of pure Bi appear after heating, pointing to the presence of significant Bi diffusion (Figure 1(c)). EELS chemical quantification reveals that the NWs average doping decreases to 1 at. % of Bi after heating. A decrease in the unit cell lattice parameter can be detected both by PXRD analysis and STEM images, suggesting that Bi is coming out of solution in a thermally activated process. In fact, a pure Bi phase is detected after the annealing, associated with Bi nucleation on external surfaces and also at grain boundaries. Indeed, high angle annular dark field (HAADF) images show the early stages of Bi nucleation, coming out of solution from the Cu cubic matrix along the edges of the NWs, indicating preferred orientations for Bi segregation during heating (Figure 1(d)). Density-functional theory will be used to explain these processes, which must be taken into account when trying to understand the behavior of these nanosystems under working conditions in future devices exploiting SHE.

Conclusions

Our study explores Bi-doped Cu nanowires grown via electrochemical deposition. Synchrotron and Advanced microscopy techniques reveal structural details critical for spin transport optimization. In-situ heating experiments expose a temperature-induced Bi diffusion, leading to nucleation of a pure Bi phase. This suggests a thermally activated process affecting NW doping and lattice parameters. Understanding these phenomena is crucial for developing efficient spintronic devices driven by the spin Hall effect.

Graphic:

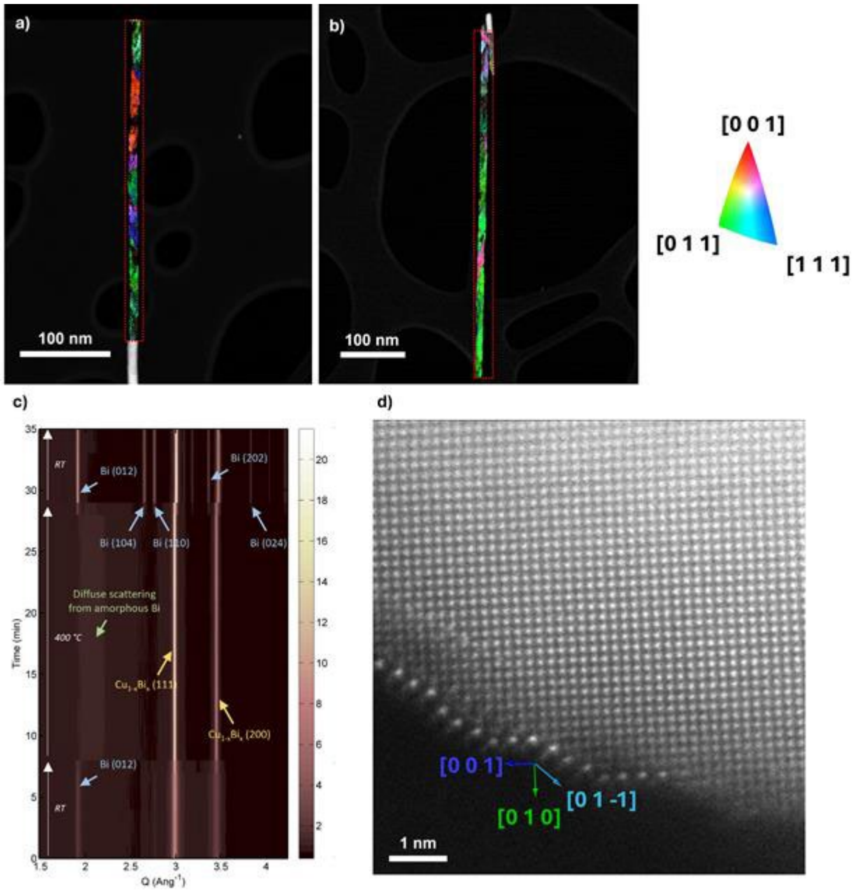

Figure 1: HAADF images and 4DSTEM out-of-plain orientation maps with a false color stereographic projection of the [001], [011] and [111] directions. (a) Small grain-like and (b) large grain-like NWs with grain sizes of around 200 nm and 1 µm, respectively. (c) Contour plot of low Q-range of time-resolved synchrotron PXRD data collected on a $Cu_{1-x}Bi_x$ (x=0.06) NW before, during and after heating to 400 °C. (d) High resolution HAADF-STEM image of the surface of a NW showing Bi segregation after heating and recrystallisation.

Keywords:

HR-STEM, EELS, in-situ, nanowires, spintronics

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