Comment on "Habit and morphology of copper precipitates in silicon"

L. Fiermans and J. Vennik

Laboratorium voor Kristallografie en Studie van de Vaste Stof, Rijksuniversiteit Gent, Krijgslaan 271, B-9000 Gent, Belgium

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The morphology of copper precipitate colonies in silicon is determined completely by a dislocation climb and glide mechanism. Interstitial dislocation loops, originating from three-dimensional nucleation centers are involved. Preferential climb in ⟨110⟩ directions of the ⟨100⟩ oriented edges of interstitial loops parallel to {110} planes and with $b=\langle 110\rangle$ determines the orientation of the colonies. The memory effect is ascribed to lattice defects which remain after complete out-diffusion of the copper.

The mechanism of formation of agglomerates of copper precipitates in silicon is known in more detail than would follow from the paper by Hu and Poponiak.[1] It leaves little doubt that copper precipitation occurs in the trails of climbing dislocations. Precipitation of interstitial impurities such as copper requires a high concentration of vacancies, not normally present in bulk material. Dislocation climb is the only mechanism capable of producing sufficient vacancies within the quenching time and copper thus will precipitate preferentially at the nonpinned parts of grown-in dislocations or at freshly formed dislocations.

During quenching, fresh dislocation loops can be created at three-dimensional defects by indentation of the matrix. Oxygen- and carbon-containing precipitates, present in the as-grown material or introduced during thermal treatments applied before copper decoration, have been proposed as indentation centers.[2–4] Nes and Washburn[5–7] suggested that the nucleation centers (SiO_2) might already be surrounded by loops before quenching. Whatever the nucleation mechanism of the fresh loops might be, copper is seen to precipitate behind climbing edge dislocations emanating from a nucleation center.

In the indentation model, the configuration of the stress field around the precipitate determines the planes in which dislocation loops will be created, favoring fully developed rosettes at isolated precipitates and swords (or ED's) on edge dislocations.[2] The preferential climb direction of the freshly formed loops further determines the morphology of the copper-precipitate colonies. Loops in {110} planes, with a ⟨110⟩ Burgers vector and consisting mainly of edges in ⟨100⟩ and ⟨110⟩ directions are thought to be involved. In order to explain the orientation of the swordlike agglomerates, e.g., parallel to {110} planes and pointing in the ⟨110⟩ directions of these planes[3] it was proposed that the ⟨100⟩-oriented edges of the loops would climb more readily than the ⟨110⟩.[2–4] An argument in favor of the preferential climb of these ⟨100⟩ edges is found in the fact that they only present one broken or rearranged bond per atom whereas this number is two for the ⟨110⟩-oriented edges.[8]

Recent investigations by Nes and Washburn[5–7] clearly demonstrate the climb-precipitation mechanism. These authors studied the morphology of microcolonies mainly by TEM. The interstitial loops parallel to {110} planes, with ⟨110⟩ Burgers vectors, which they observed surrounding the colonies, in our opinion would give rise to swordlike patterns in the case of heavily copper-doped material. As they did not dope their samples intentionally however, other fast-diffusing impurities might be involved, possibly giving rise to the {100} branches. The latter clearly are not formed by the same mechanism as the {110} branches. It should be mentioned that the {100} branches have not been observed consistently in heavily copper-doped silicon. The impurities involved could be iron or nickel. Unfortunately these impurities interact with oxygen, carbon, and vacancy clusters in a less well-known manner. It seems nevertheless established that dislocation climb is not essential for their precipitation.

From the photographs published by Nes and Washburn it can also be seen that the morphology of the copper specs themselves is not relevant since after their formation they do not contribute any further to the growth of the colony.

As far as the memory effect mentioned by Hu and Poponiak is concerned, it is felt from our experiments[2] that after the out-diffusion of the copper the original dislocations or tangles remain in essentially the same configuration. Furthermore, a high concentration of collapsed vacancy disks might be introduced within the swords if the out-diffusion proceeds too rapidly to allow the vacancies to be absorbed by dislocations or by the free surface. Macroscopically, the stress field due to these imperfections is liable to produce approximately the same x-ray contrast as with the precipitates still present. Experimentally, this was found to be true. After complete removal of the copper, x-ray topography still gave identical images with only a slightly reduced intensity, whereas ir microscopy showed precipitate-free samples. It would be very instructive to study the exact nature of the remaining defects by means of TEM.

It should finally be pointed out that the Si-SiO_2 interface is a boundary for dislocation climb, giving rise to the truncated ED's observed by Hu and Poponiak.[1] It would follow also that the interface is only a minor sink for copper since no depleted region has been observed as for the free surface and that no fresh dislocations are introduced at the interface.

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