Formation of BCC-Cu_3Si in CZ-Si

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With increasing use of metal Cu in Si device processes, control of the Cu impurity becomes of emergent importance, because it is a fast diffusive species among various impurities and causes degradation of devices. Cu can precipitate and act in silicide particles with a large structural variety, which is dependent on annealing temperature, quenching rate, doping, and presence of other extended defects. This paper reports the formation of novel copper silicides with a body-centered cubic (BCC) structure, which is not the thermal equilibrium η structure observed previously in Cu-doped Si [1], in Czochralski (CZ) grown Si crystals heavily doped with p-type dopant atoms.

When Cu atoms were doped, planar defects about 5 nm in thickness, laid on nearly {112}, were formed in CZ-Si doped with p-type dopant atoms (B or Ga atoms with the concentration up to $10^{20}cm^{-3}$), irrespective of dislocations. The planar size increased with increasing the concentration of p-type dopant atoms (up to a few tenth μm). The defects were not formed in heavily B-doped Si grown by the floating-zone (FZ) method and in CZ-Si doped with n-type dopant atoms (P, As, Sb). These results indicate that the defects were formed in Si including oxygen and p-type dopant atoms.

The defects were agglomerates of Cu_3Si nanocrystals with a BCC structure (a=0.285 nm), revealed by high resolution transmission electron microscopy combined with energy dispersive x-ray spectroscopy. The interface between a nanocrystal and the host Si crystal was of a sigma-3 type. It is theoretically suggested that a Cu_4 cluster, one substitutional Cu atom associated with three neighboring interstitial Cu atoms, is formed in Si [2], and the nucleus of the BCC-Cu_3Si nanocrystals may be the agglomerate of four Cu_4 clusters. Actually, we have shown that Cu atoms tend to form the BCC-Cu_3Si structure in Si rather than to dissolve in Si, by ab-initio calculations.

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