

## Work function of Cu<sub>3</sub>Ge thin film

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Cu<sub>3</sub>Ge is one of the best alternatives to Cu for contacts/ interconnections in microelectronics industry, owing to its thermal stability up to 450 °C [1, 2] and low bulk resistivity ( $\sim 8 \pm 2 \mu\Omega \text{ cm}$ ) over a large Ge composition range of 25-35 at.% [1, 3]. The out diffusion of Cu is suppressed [4], such that diffusion barrier is no longer needed and the service life of interconnects can be improved considerably. In addition, Cu<sub>3</sub>Ge remains stable against oxidation in air up to  $\sim 500$  °C [4, 5]. Consequently, Cu<sub>3</sub>Ge has been considered superior to Cu as contacts/ interconnections for integrated circuit devices. Despite the remarkable progress, the reported Cu<sub>3</sub>Ge films were frequently polycrystalline with excess Ge. Epitaxial Cu<sub>3</sub>Ge film is highly desired owing to reduced diffusion paths and possibly lower electrical resistivity. Therefore can epitaxial Cu<sub>3</sub>Ge thin film be fabricated and what are its electrical properties? Here, we present the fabrication of epitaxial Cu<sub>3</sub>Ge thin film and its work function, characterized by Kelvin probe force microscopy (KPFM). The average work function of epitaxial Cu<sub>3</sub>Ge thin film is measured to be  $\sim 4.47 \pm 0.02$  eV, rendering it a desirable mid-gap gate metal to be used for CMOS devices because it requires minimal and symmetric channel implants even at linewidths below 0.5  $\mu\text{m}$  [6].

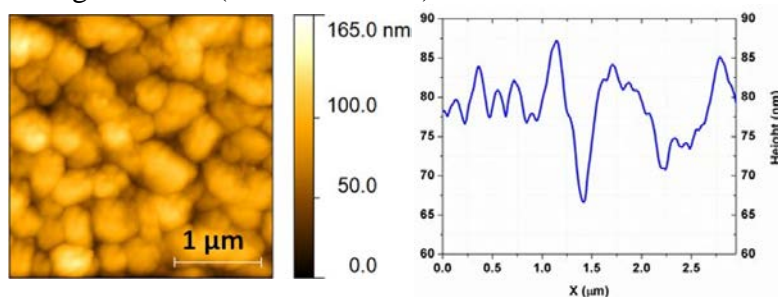
In order to obtain epitaxial Cu<sub>3</sub>Ge thin films, 5 samples were fabricated on c-sapphire substrate by controlling the deposition parameters of pulsed laser deposition (PLD). 90 thin layers of Cu and Ge (thus a total of 180 layers) were deposited alternatively on c-sapphire for each sample. The laser pulse numbers in each repetition of Cu and Ge ablations from sample 1 to 5 are 35:5, 25:5, 15:5, 14:2 and 7:1. The laser exciting voltage was maintained at 23.8 keV (according to previous experience in PLD deposition [7-13]). The XRD  $\theta$ -2 $\theta$  patterns of samples 1-3 show Ge (111) peak (@ 27.32°), indicating the existence of excess Ge. In contrast, pure Cu<sub>3</sub>Ge thin films were obtained for samples 4 and 5, as evidenced by the disappearance of Ge peak. However, the obtained Cu<sub>3</sub>Ge thin film is still polycrystalline for sample 4, due to the existence of Cu<sub>3</sub>Ge {002}, {020}, {-111} peaks. Only Cu<sub>3</sub>Ge {002} and {020} peaks exist in the XRD  $\theta$ -2 $\theta$  pattern of sample 5, indicating a bi-epitaxial relationship between the Cu<sub>3</sub>Ge thin film and the c-sapphire substrate. Since only 1 pulse was used to ablate each Ge layer, this should be the optimum condition for epitaxial Cu<sub>3</sub>Ge thin film fabrication by PLD.

Work function is a fundamental electronic property of a metallic surface, affecting both electron emission through the surface and electronic trajectories near the surface [14]. The local work function of epitaxial Cu<sub>3</sub>Ge thin film  $\phi_{\text{Cu}_3\text{Ge}}$  was measured by KPFM. KPFM measures the work function of solid surfaces at atomic or molecular scales, demonstrating information about composition and electronic state of the local structures on the surface. When the conducting tip and the sample are brought in contact, a net electric current would flow between them until the Fermi levels were aligned. During measurement a voltage is applied between tip and sample, consisting of a DC-bias and an AC-voltage. When  $V_{\text{CPD}}$  (the contact potential difference between a conductive tip and a sample) =  $V_{\text{DC}}$  (the applied DC voltage on the tip), the electrostatic force component measured at frequency  $\omega$  and the oscillating amplitude would be zero. Consequently  $V_{\text{DC}}$  can track  $V_{\text{CPD}}$  at each point of the scan area by using a feedback circuit. Once  $V_{\text{CPD}}$  is obtained, the local work function of Cu<sub>3</sub>Ge thin film  $\phi_{\text{Cu}_3\text{Ge}}$  can be calculated as the difference of  $\phi_{\text{tip}}$  (work function of the conductive tip,  $\sim 4.90 \pm 0.02$  eV [15]) and  $eV_{\text{CPD}}$ .

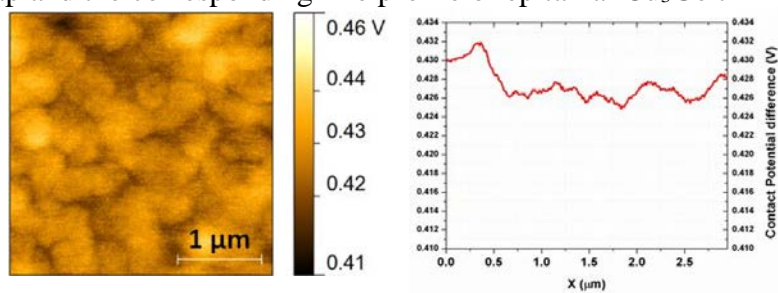
Although small grains of tens of nanometers can be seen from the topographical image, an almost uniform distribution of  $V_{\text{CPD}}$  within each grain was observed from the contact potential image. Figure 1 and 2 show the topographical and surface potential images for epitaxial  $\text{Cu}_3\text{Ge}$  thin film, and the corresponding line profiles derived from them, demonstrating the height and  $V_{\text{cpd}}$  variation. The average  $V_{\text{CPD}}$  for epitaxial  $\text{Cu}_3\text{Ge}$  thin film was measured to be  $\sim 0.43$  V. Therefore the work function of  $\text{Cu}_3\text{Ge}$  thin film is  $\sim (4.47 \pm 0.02)$  eV, which is between the work functions of  $n^+$  and  $p^+$ -polysilicon [6]. This value is desirable for epitaxial  $\text{Cu}_3\text{Ge}$  thin film to be used as a mid-gap gate metal even at very low temperatures for applications in CMOS devices, because it would require minimal and symmetric channel implants even at linewidths below  $0.5\mu\text{m}$  [6].

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**Figure 1.** Height map and the corresponding line profile of epitaxial  $\text{Cu}_3\text{Ge}$  thin film.



**Figure 2.** Surface potential map and the corresponding line profile of epitaxial  $\text{Cu}_3\text{Ge}$  thin film.