The growth of pinhole-free epitaxial $RESi_{2-x}$ thin films on atomically clean Si substrates

W. C. Tsai, K. S. Chi, and L. J. Chen

Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, Taiwan, Republic of China

Rare-earth (RE) metal silicides have received much attention for both fundamental and technological reasons. The excellent lattice match between the RE silicides of hexagonal AlB_2 structure and Si substrates offers an opportunity to grow high-quality epitaxial silicides on silicon. The metallic resistivity and low Schottky barrier height (0.3-0.4 eV) on n-type Si are particularly attractive for electronic applications.

Various defects were found to form in RE silicides on silicon. Extensive studies on the formation of pinholes have been carried out. Many methods to overcome this problem, and mechanisms for pinhole formation, have been reported. In this paper, we report the growth of pinhole-free $RESi_{2-x}$ thin films. The mechanism for pinhole formation is discussed.

Thin metal films (Y or Yb), 30 nm in thickness, were deposited on (111) and (001)Si substrates in an ultrahigh vacuum electron beam evaporation chamber at a substrate temperature of 500 ^{o}C. Various thicknesses of amorphous Si were deposited onto the metal layers. *In situ* UHV annealing was carried out immediately after thin film deposition at room temperature. Transmission electron microscopy (TEM) analysis was carried out with a JEOL-2010 TEM operating at 200 keV. Surface morphology was examined by a HITACHI S-4000 scanning electron microscopy (SEM) equipped with a cold cathode field emission gun operating at 15 keV.

A high density of pinholes was found to form in epitaxial YSi_{2-x} thin films. The pinholes are rather difficult to be annihilated by high temperature annealing once they are formed. Based on the experimental findings, the Stranski-Krastanov growth behavior of epitaxial $RESi_{2-x}$ thin films on Si by solid phase epitaxy leads to the random formation of a high density of pinholes.

The growth of pinhole free epitaxial $YbSi_{2-x}$ and $ErSi_{2-x}$ thin films on (111)Si was carried out by capping *a*-Si layer with appropriate thickness before subsequent annealing. The density and the size of pinholes were found to decrease and increase, respectively, with the thickness of the capping layer. Appropriate thickness of *a*-Si capping layer is necessary to grow pinhole-free epitaxial $RESi_{2-x}$ films on Si substrates. As a result, pinholes can be avoided by appropriate fabrication process.