Abstract No. jord0551

Evolution of Texture in TiSi Thin Films

A. Özcan, K. Ludwig, Jr. (Boston U.), C. Lavoie, C. Cabral, Jr., and J.M.E. Harper (IBM)

Beamline(s): X20C

Introduction: Texture (preferential crystallite orientation) evolution in titanium silicide thin films was investigated and the mechanisms of silicide phase formation studied. Titanium disilicide ($TiSi_2$) thin films, formed by reactions between titanium and silicon, have received a great deal of interest because of the material's wide use in integrated circuits as contact electrodes. Titanium disilicide exists in two polymorphs, both orthorhombic, with crystallographic designations C49 and C54. Although the technologically preferred low-resistance C54 phase is the equilibrium structure, the C49 phase is kinetically favored under most conditions. The transformation to the C54 phase can be difficult due to the small free energy difference between the two phases. One of the promising methods developed to enhance the formation of the C54 is addition of a refractory metal (such as tantalum (Ta), molybdenum (Mo)) to the initial titanium film, either by alloying with the refractory metal or by depositing a thin layer between the titanium film and the substrate.

Methods and Materials: In order to better understand the fundamental mechanisms governing the C54 phase formation, texture formation in $TiSi_2$ thin films with and without Ta addition has been systematically examined.

Results: Detailed orientational studies (x-ray pole figure analysis) of the pure C54 phase films on Si(001) substrates suggest that the C54 texture can be related to preferential nucleation on Si<111> microfacets, which possibly form earlier during the C49 nucleation. Three prominent C54 orientations were identified and their evolution was further examined using synchrotron based time-resolved *in-situ* x-ray diffraction. Significant differences were observed in the kinetics of individual orientations. On the other hand, analysis of the kinetics for different temperatures implies the presence of a limited number of C54 nucleation sites.

Silicide formation is also studied in Ti films alloyed with Ta and in films with Ta interlayers between the Si and the Ti. These studies show that the enhancement of the C54 phase in these cases may be related to the development of a strong (010) texture. The mechanisms responsible for the texture change and its implications are discussed in the references.

References:

A. Özcan, "Evolution of Texture in TiSi Thin Films," Ph.D. Thesis, Boston University, MA, USA, 2002.
A. Özcan, K.F. Ludwig, C. Lavoie, C. Cabral, Jr., J.M.E. Harper, J. Appl Phys, **92**, 5189 (2002).
A. Özcan, K.F. Ludwig, P. Rebbie, C. Cabral, Jr., C. Lavoie, J.M.E. Harper, J. Appl Phys, **92**, 5011 (2002).