GROWTH KINETICS AND ELECTRONIC PROPERTIES OF MOLYBDENUM BASED SILICIDES

By

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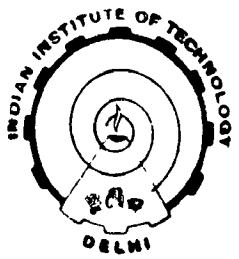
DEPARTMENT OF PHYSICS

Thesis submitted in fulfilment
of the requirements of
the degree of
DOCTOR OF PHILOSOPHY



to the

INDIAN INSTITUTE OF TECHNOLOGY, DELHI

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Dedicated

to

my beloved father

who inspired me for my scientific endeavor

and

my mother

who provided me moral and emotional support

CERTIFICATE

We are satisfied that the Thesis entitled "**Growth Kinetics and Electronic Properties of Molybdenum Based Silicides**" presented by Ravi Shankar Rastogi is worthy of consideration for the award of the Degree of Doctor of Philosophy and is a record of the original bonafide research work carried out by him under our guidance and supervision, and that the results contained in it have not been submitted in part or full to any other university or institute for the award of any degree/diploma.

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ABSTRACT

The present research work elucidates the information on growth kinetics and electronic properties of molybdenum disilicide and solid state interaction of co-sputtered amorphous and polycrystalline $MoNi_x$ alloys, and bilayer structures of Mo/Ni and Mo/Co with silicon. Structural transformation during rapid thermal annealing of co-sputtered $MoSi_x$ alloys has been investigated by glancing angle X-ray diffraction. The results indicate the formation of $MoSi_2$ phase as the first phase of nucleation at as low as ~ 700°C. The grain growth kinetics of $MoSi_2$ has been studied by measuring the grain size and sheet resistance measurements in isochronal annealed samples using Arrhenius relation. The effect of oxygen contamination on the growth (structural transformation) and surface morphology of $MoSi_2$ has also been investigated. Due to oxygen contamination, a mixture of Mo_5Si_3, $MoSi_2$ and Si phases is obtained at as low as 700°C and is converted to $MoSi_2$ tetragonal phase at ~1150°C. AES and XPS studies reveal that $MoSi_2$ has a mixture of covalent and metallic bonds and is predominated by covalent nature of bonds. EELS investigations in valence and core level provides the knowledge of various new interband transitions from valence and core level to E_F or above E_F due to silicide formation. Using the two EELS and

XPS data, a tentative energy band diagram is proposed for $MoSi_2$.

Investigations on interaction of polycrystalline $MoNi_x$ alloys show a reaction between the alloy and silicon at ~ 500°C due to depletion of nickel. In amorphous alloys, molybdenum rich alloys were found to be stable on silicon up to ~500°C and do not react with it. While nickel rich alloys react with silicon at the same temperature due to out-diffusion of nickel from $MoNi_x$ alloy. Various reaction mechanisms have been observed to follow in these alloys-silicon interaction and are explained on the basis of silicide formation temperatures, nature of diffusing species, metal-metal interaction, lower interfacial energy and solid solubility . In molybdenum rich amorphous and polycrystalline alloys, the reaction is dominated by the in-diffusion of silicon into the alloy while in nickel rich amorphous and polycrystalline alloys, the reaction occurs mainly due to out-diffusion of nickel from the alloy. In all the polycrystalline and amorphous alloys, a macroscopic phase separation phenomenon is observed at different temperatures and has a layer structure of $MoSi_2$+NiSi($NiSi_2$)/NiSi($NiSi_2$)/Si(Xtal).

In Mo/Ni/Si (Xtal) and Mo/Co/Si (Xtal) bilayer structures, the effect of interposed nickel and cobalt layers was found to lower the silicide formation temperature

between 500 and 550°C, supress the effect of interfacial impurities and smoothen the surface morphology of $MoSi_2$ films. The reaction kinetics is discussed on the basis of diffusing species (Ni, Co and Si) at low temperature. The presence of nickel and cobalt enhances the rate of silicide formation. The resulting smooth surface morphology has been explained by considering the role of stresses.

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