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Effect of temperature on microstructure and electrical properties of $TaSi_2$ thin films grown on Si substrates

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ABSTRACT

Tantalum silicide ($TaSi_2$) thin films were deposited on n-type silicon single crystal substrates using a dual electron-gun system and with Ta and Si targets. The thicknesses of $TaSi_2$ thin films considered in this study are in the range 200–500 nm, respectively. The $TaSi_2$/Si samples were annealed at temperature 1173 K for 2 h in a vacuum of 10^{-8} mbar. The structure of the tantalum silicide thin films was investigated by X-ray diffraction (XRD). X-ray diffraction results show changes in the structure of $TaSi_2$ thin films from amorphous to crystalline after annealing. According to XRD analysis, a complete conversion to single-phase disilicide $TaSi_2$ was achieved from a sample composition of Ta:Si = 1:2. DC conductivity was measured for the $TaSi_2$ thin films in the temperature range 300–900 K before and after annealing. It has been observed that the DC conductivity and activation energy was affected by changing the $TaSi_2$ film thickness and by annealing. The experimental results indicate that, the conduction phenomena of the investigated sample proceeded via two distinct mechanisms. The first one in the low-temperature range $T < 500$ K can be described by thermally-assisted tunneling of the carriers in the localized states near the band edge. The value of the pre-exponential factor before and after annealing is less than $10^4\ \Omega^{-1}\ cm^{-1}$. The other process appears in the high temperature region $T > 500$ K, where thermally activated conduction occurs through the extended states. Here the value of the pre-exponential factor before and after annealing is larger than $10^4\ \Omega^{-1}\ cm^{-1}$. The conductivity is greater in the crystalline phase than in the amorphous phase. The activation energy ΔE for our films before and after annealing is increased with increasing film thickness.

1. Introduction

The refractory metal silicides, such as, WSi_2, $TaSi_2$, $MoSi_2$ and $TiSi_2$ are becoming useful gate and interconnect materials in very large scale integrated circuits (VLSI) [1–3]. Refractory metal silicides have been studied intensively because of their importance in the semiconductor industry. The low resistivity and an excellent chemical stability make them one of the attractive materials for interconnections and low resistance contacts in integrated circuits [4]. They are used as protective layers against oxidation on metallic surfaces at high temperatures [5]. Among the metal silicides, $TaSi_2$ has higher temperature stability and low contact resistance. The most interesting point of $TaSi_2$ is that it can be directly used as a gate material without need for ploy-Si [6,7]. Silicide layers for electronics were recently summarized in the book of Wetzig and Schneider [8].

Silicide films can be made by direct deposition [9,10] or by reaction of metal films on silicon substrates [11,12]. It has been found that Ta and Si react very rapidly to form $TaSi_2$ at temperature >900 °C [13].

The present study and investigation of the film $TaSi_2$ was undertaken with three different aims in mind. First, one hoped to contribute some improved understanding of the metallurgy of the silicide. More specifically, one wished to explore the effect of several processes of heat treatment on the conductivity of the film. A final goal was to explore possible relationships between the structure and the resistivity of $TaSi_2$ films.

Several workers [14] have reported the structural properties Ta–Si layers with different compositions. In the present work, the electrical and structural properties of stoichiometric $TaSi_2$ films with different thicknesses and at different temperatures have been studied.

2. Experimental details

Thin films of $TaSi_2$ alloys were prepared by simultaneous evaporation of the components (Ta and Si) in a UHV double electron-gun evaporation system [15]. The UHV was provided with

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a titanium sublimation pump and circulating liquid N_2. Approximately 2 min before opening the shutter the evaporation process was started the pressure, which was in the lower 10^{-9} mbar range before evaporation, rose to approximately 5×10^{-8} m bar during this process. Formation of stoichiometric $TaSi_2$ on Si-single crystal substrates requires as-deposited films with a Ta:Si thickness ratio of 1:2, which takes into account material densities [4]. The thickness was measured with a quartz monitor, whose tooling factors had to be calibrated from direct x-TEM measurements of the layer widths [16]. The deposited film thicknesses were in the range 200 nm–500 nm. The Si-substrates (100) n-type dipped in white etch and buffered HF before deposition. The deposition parameters where kept almost same for all the samples so that a comparison of results could be made for various sample thicknesses.

The thin film nature of the samples was examined by X-ray diffraction using the diffractometer with Cu Kα radiation source ($\lambda = 1.54$ A°). This investigation was made for the films before and after annealing at temperature 1173 K for 2 h. X-ray diffraction (XRD) was used to analyze the phase formation in the films.

For DC conductivity measurements, the samples were mounted in a specially designed metallic sample holder where a vacuum of about 3×10^{-4} m bar could be maintained throughout the measurements.

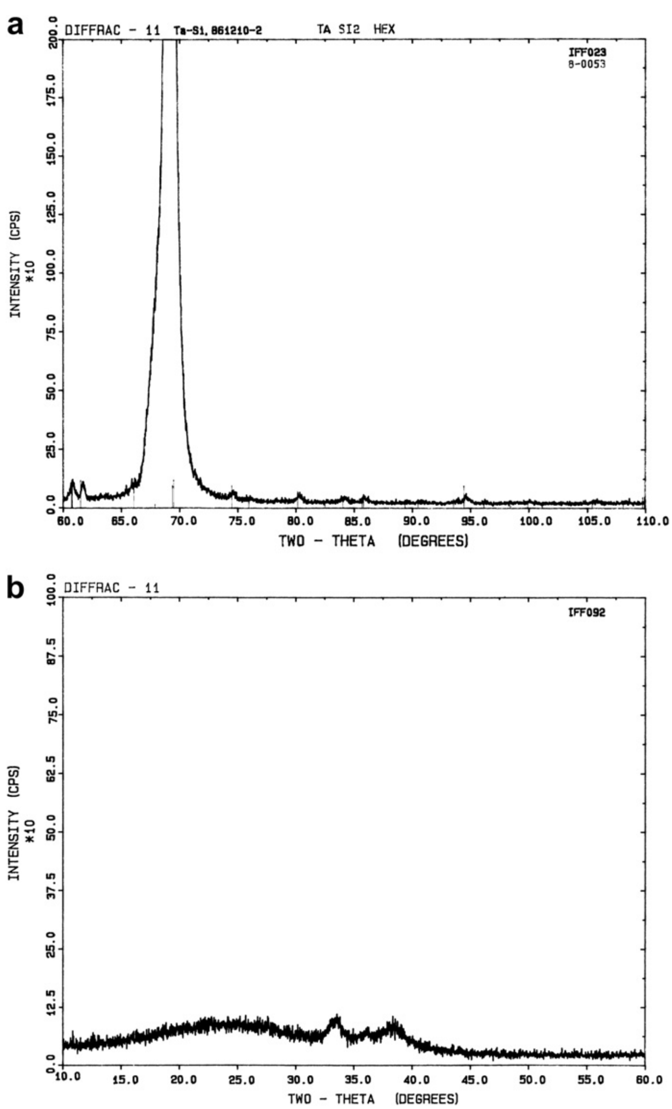

Fig. 1. XRD for: (a) the substrate and (b) the thin film before annealing.

A voltage (1.0 V) was applied across the sample and the resulting current and the sample resistance R_s were measured by a digital electrometer (Keithley, model 617). The temperature was measured by mounting a calibrated copper–constantan as thermocouple near the sample. The electrical conductivity was measured for the samples of different thicknesses before and after annealing in the temperature range 300–900 K in vacuum.

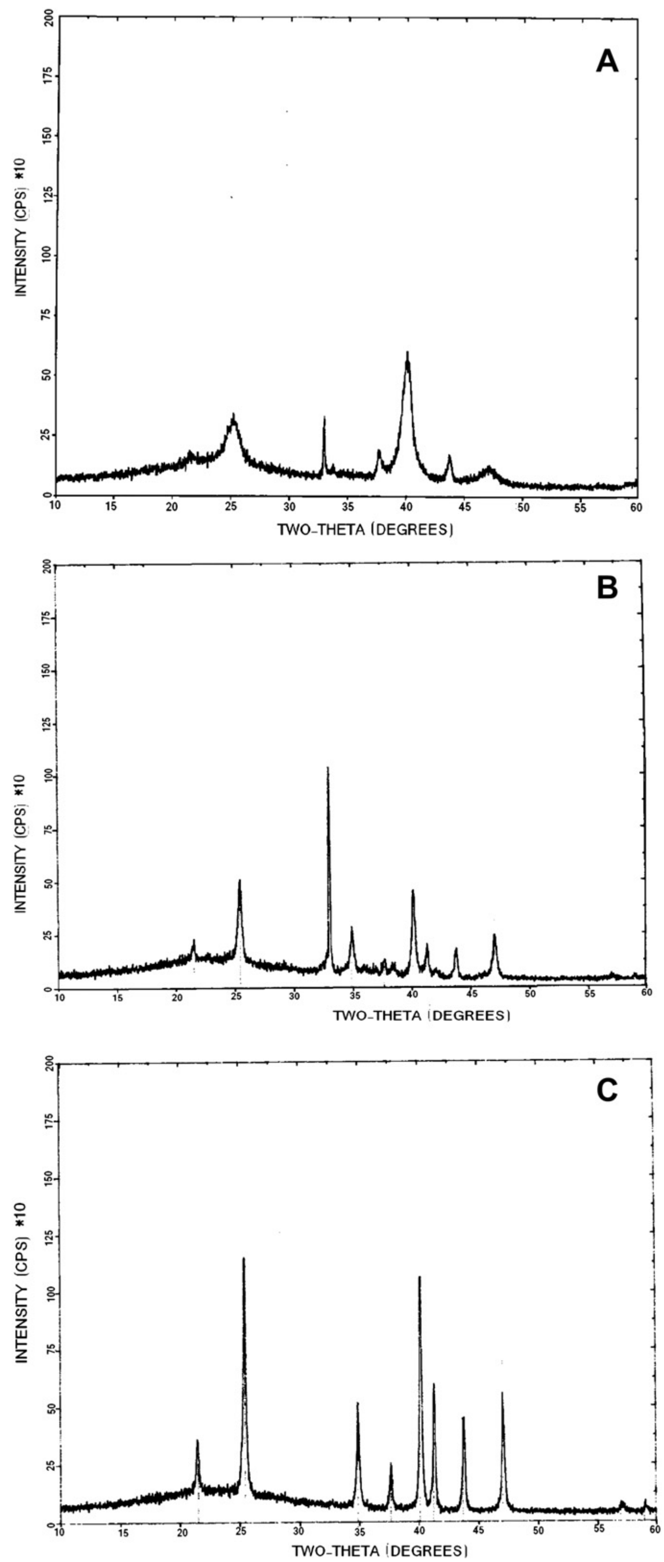

Fig. 2. XRD for the film after annealing for: (A) 10 min (B) 15 min. and (C) 2 h.