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Cobalt silicide formation on 6H silicon carbide

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Cobalt films (1, 25 and 100 Å) have been directly deposited on top 6H-SiC(0001) wafers by molecular beam epitaxy and annealed at 500-800°C in UHV. The structure of the metal-semiconductor interface was investigated by XAFS. The results show that Co-Si bonds were preferentially formed in the 1 Å Co films. In the 25 and 100 Å Co films only Co-Co bonds were identified. The XRD pattern of the 100 Å Co film exhibits a Co (200) peak confirming the presence of unreacted metal even after annealing at 800°C.

keywords: Silicon Carbide; metal-semiconductor contacts;molecular beam epitaxy.

1. Introduction

Silicon Carbide (SiC) devices have been extensively used in high temperature and high power environments. For those applications the development of stable metal contacts is required. High quality $CoSi_2$ films have been used as contacts in silicon devices. This silicide has low resistivity (~ 15 μΩ.cm) and high chemical stability and it is a natural candidate for a contact material for SiC devices.

The published information about the morphology and chemical structure of Co/SiC interfaces is relatively incomplete. For Co samples directly deposited on carbon terminated surface of 6H-SiC(0001) only the formation of a CoSi-type structure after annealing at 900°C has been reported (Lundberg *et al.*, 1994). Further annealing of the films (1350°C) did not reveal any $CoSi_2$. Similar results were obtained by Porter *et al.* (1995) for 1000 Å-thick Co films deposited on 6H-SiC, where cubic CoSi was the only phase detected after annealing at 1000°C. According to published results (Nathan *et al.*, 1991), in this metal-semiconductor interface Co_2Si is formed at temperatures between 400-1200°C. The reaction proceeds to CoSi and then to the formation of the $CoSi_2$.

The understanding of the chemical structure and morphology of this interface is fundamental for the dedevelopment of high quality Co contacts to SiC.

2. Experimental

Co films were prepared on 6H-SiC(0001) wafers, n-type, N-doped purchased from Cree Research, Inc. The wafers were exposed to the UV/ozone irradiation and then chemically etched with a HF:H_2O:ethanol (1:1:10) solution. After this cleaning procedure the wafers were thermally desorbed at 850°C in UHV under Si flux for 10 minutes. After thermal desorption a 1x1 LEED pattern was observed. Auger spectra showed a sharp Si peak (92 eV) characteristic of a clean SiC silicon terminated surface. Thin Co films (25 and 100Å) were then deposited in UHV followed by thermal annealing for 20 minutes at 600-800°C. *Ex situ* XAFS measurements were performed at room temperature in fluorescence mode at the Co-K edge.

The 1 Å Co film was deposited on a SiC wafer previously cleaned as described above, in a system composed of a deposition and an analytical chamber installed at beamline X-11A at the NSLS (Sayers *et al.*, 1998). The deposited materials can be studied *in situ* with RHEED, XAFS and AES. XAFS data of the film were collected at room temperature, 500°C and 800°C in total electron yield mode at the Co K-edge.XAFS data treatment (Sayers & Bunker, 1998) was performed with MacXAFS and the structural parameters were extracted by a non-linear fitting procedure. Experimental phases and amplitudes were used to fit the data.

X-ray diffraction (XRD) measurements of the 100 Å Co films were performed in the θ-2θ mode with Cu K_α radiation on a Rigaku Geigerflex diffractometer with a (0001) graphite monochromator.

3. Results and Discussion

The Fourier Transforms (FT) of the k^2-weighted XAFS data are shown in Figs. 1 to 3. The FT of k^2-weighted XAFS data was performed over a k range of 3.3-8.9 $Å^{-1}$, and the inverse of FT was taken over 1.35-3.01 Å. For the 1 Å Co films (Fig. 1) only one coordination shell was observed in all measurements. The shell consisted entirely of Si atoms at 2.34 Å . Therefore we conclude that in this film Co reacts with the substrate at room temperature. The Co-Si coordination number and bond lenght remained constant at approximately 4.2 and 2.34 Å, respectively, after annealing at 500°C and 800°C, which indicates the formation of a CoSi- type structure._In the CoSi structure there are 4 Co-Si, 3 Co-Si and 6 Co-Si at 2.33 Å, 2.47 Å and 2.73 Å, respectively. The Debye-Waller factor decreases with increasing annealing temperature, which is consistent with the presence of spots characteristic of island formation at 800°C. For the 25 Å (Fig. 2) and 100 Å (Fig. 3) Co films the Fourier transforms also show only one coordination shell. The shell consisted entirely of Co atoms. As can be seen in Table 1, the estimated coordination number (≈10.0) and bond distance (≈2.50 Å) values are similar to those obtained for metallic Co at room temperature. These results show that the deposited metal remains unreacted even after annealing at 800°C.

XRD patterns obtained for the 100 Å Co films annealed at 600, 700 and 800°C (Fig.4) show the presence of a (200) Co diffraction peak, confirming that Co did not react with the SiC substrate.

The presence of unreacted Co in the 25 and 100 Å Co films may indicate that longer annnealing times will be required, in the case of thicker Co films, to form CoSi and $CoSi_2$. Since SiC material is transparent in the Infrared region the radiactive heat transfer may not be efficient and the actual temperature may be lower than expected. The lack of CoSi formation in the 25 and 100 Å films may be in part due to such inefficient heating.

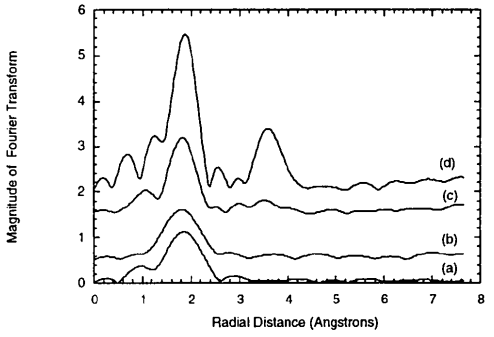

Figure 1
Fourier transform of k^2-weighted XAFS data for 1 Å of Co deposited on 6H-SiC and annealed at 500°C (a), 600°C (b) and 800°C (c) and $CoSi_2$ (d).

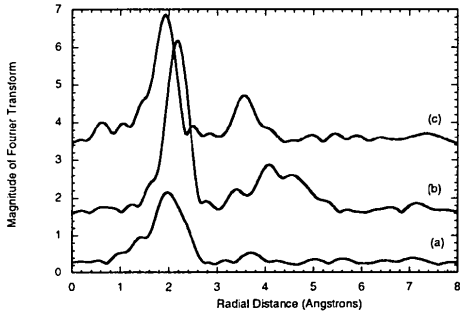

Figure 2
Fourier transform of k^2-weighted XAFS data for 25 Å of Co deposited on 6H-SiC and annealed at 800°C (a), Co foil at room temperature (b) and $CoSi_2$ (c).

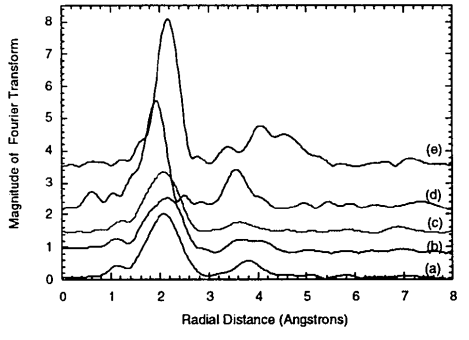

Figure 3
Fourier transform of k^2-weighted XAFS data for 100 Å of Co deposited on 6H-SiC and annealed at 600°C (a), 700°C(b), 800°C (c), $CoSi_2$ (d) and Co foil at room temperature (e).

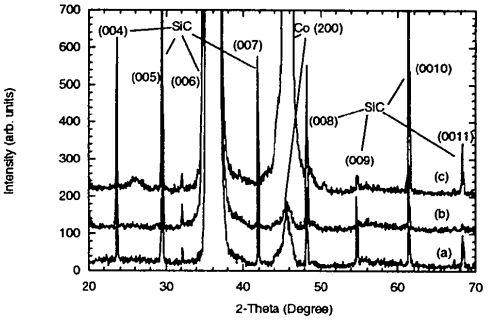

Figure 4
XRD scans of 100 Å Co films deposited on 6H-SiC (0001) and annealed at 600°C (a), 700°C(b) and 800°C(c).

Table 1
Coordination numbers, N_j, bond lenght,R_j, and Debye Waller factor, σ^2_j, for Co/SiC samples. L and B are, respectively, the Co thickness and neighboor. The estimated N_j, R_j and σ^2_j errors are ± 0.5, ± 0.01 Å and ± 0.0001, respectively.

L (Å)	B	T (°C)	N_j	R (Å)	$\Delta\sigma$ (Å^2)
1	Si	25	4.7	2.36	0.0078
	Si	500	4.7	2.34	0.0080
	Si	800	4.6	2.34	0.0029
25	Co	800	10.6	2.50	0.0140
100	Co	600	9.8	2.51	0.0110
	Co	700	10.1	2.50	0.0106
	Co	800	11.0	2.51	0.0121
Co-foil	Co	25	12.0	2.50	0.0070

4. Conclusions

The results showed that a CoSi-type structure was formed in the 1 Å Co film directly deposited on 6H-SiC at room temperature and annealed at 500 and 800°C. The presence of unreacted cobalt was identified in the 25 and 100 Å Co films directly deposited on 6H-SiC and annealed at 600-800°C. These results indicate that longer annealing times are required for the thicker films (25 and 100 Å) to form CoSi.

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References

Lundberg, N. & Ostling, M. (1994). Physica Scripta T54, 273-277.
Nathan, M. & Ahearn, J. S. (1991). J. Appl. Phys. 70, 811.
Porter, L. M., Davis, R.F., Bow, J. S., Kim, M. J. & Carpenter, R. W. (1995). J. Mater. Res. 10 (1), 26-33.
Sayers, D.E., Goeller, P.T., Boyanov, B.I. & Nemanich, R. J. (1998). J. Synchrotron Rad. 5, 1050-1051.
Sayers, D. E. & Bunker, B. A. (1998). X-Ray Absorption: Principles, Applications, Techniques of EXAFS, SEXAFS and XANES, edited by D.C.Koningsberger & R. Prins, New York: Wiley.

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