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NEW MODELS FOR OHMIC CONTACTS TO GaAs*

A. K. KULKARNI AND C. LAI
Department of Electrical Engineering, Michigan Technological University, Houghton, MI 49931 (U.S.A.)

Gold-based ohmic contacts are routinely used in GaAs devices and integrated circuits. Since either electron-beam deposited or thermally evaporated gold is in the polycrystalline form, grain boundary diffusion of gallium into gold is expected. Using sputter Auger depth profiles of electron-beam deposited and annealed gold contacts on n-type GaAs, the concentration of gallium in gold as a function of the annealing temperature (250 to 550 °C with a step of 50 °C) is determined. Applying Whipple's grain boundary diffusion theory, the grain boundary diffusion coefficient for gallium in gold layer is found to be $3.5\times10^{-9}\exp(-0.21/kT)\ \mathrm{cm^2\,s^{-1}}$. The lattice diffusivity is equal to $6.5\times10^{-13}\exp(-0.33/kT)\ \mathrm{cm^2\,s^{-1}}$. The study on gold diffusion in GaAs based on the capture of gold atoms by gallium vacancies and gold migration along interstices yielded the diffusion coefficient of gold equal to $3.12\times10^{-3}\exp(-1.59/kT)\ \mathrm{cm^2\,s^{-1}}$.

1. INTRODUCTION

Two interesting new models for ohmic contacts to GaAs based on structure-property relationships have been published recently. Based on the experimental results of Kuan *et al.*[1], the key point in the formation of low resistance ($1\times10^{-6}\ \Omega\,\mathrm{cm^2}$) ohmic contacts appears to be the diffusion of germanium from the NiGe phase to the NiAs phase to form an Ni_2GeAs phase. A second model based on gallium-vacancy-dependent diffusion of germanium has been suggested by Gupta and Khokle[2]. This model assumes grain boundary diffusion as the principal mechanism of gallium diffusion into gold. Very recently Gupta *et al.*[3], have reported quantitative data concerning the diffusion of gallium into gold.

We have reported the effect of annealing process parameters on the electrical and interfacial properties of AuGe ohmic contacts to n-type GaAs[4]. An analysis of the sputter Auger depth profile data on AuGe contacts based on grain boundary diffusion was very complicated because of intermixing of several elements of *i.e.* gold, germanium, gallium and arsenic.[5] In order to simplify the analysis and understand clearly the grain boundary diffusion mechanism we have investigated the Au–GaAs system thoroughly in this paper.

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2. FABRICATION AND MEASUREMENT

High purity (99.999%) gold was deposited to a thickness of 100 nm (as measured by a thickness monitor) by electron-beam deposition in an ultrahigh vacuum system. The GaAs substrates were silicon doped ($N = 5.2\text{–}7.2 \times 10^{17}\ \text{cm}^{-3}$) $\langle 100 \rangle$ oriented n-type substrates. The details on cleaning of the substrates and deposition process are discussed elsewhere[6]. The gold contacts were annealed at various temperatures ranging from 250 to 550 °C with a step of 50 °C, in dry N_2 for 5 minutes.

Auger sputter depth profiles were obtained on all the samples using an Auger electron spectrometer (PHI Model 545). Two computer programs were developed to amass the information collected in a series of AES spectra and generate depth–composition profile data in both tabular form and figure format[6]. Figure 1 shows a typical Auger sputter depth profile of an as-deposited (unannealed) Au–GaAs contact. As expected, an abrupt interface with less than 5% O_2 at the interface is observed. Comparing this sample with a sample annealed at 450 °C for 5 min (Fig. 2) the out-diffusion of gallium to the surface and indiffusion of gold into GaAs are clearly seen. The gallium on the surface appears to be in the form of gallium oxide.

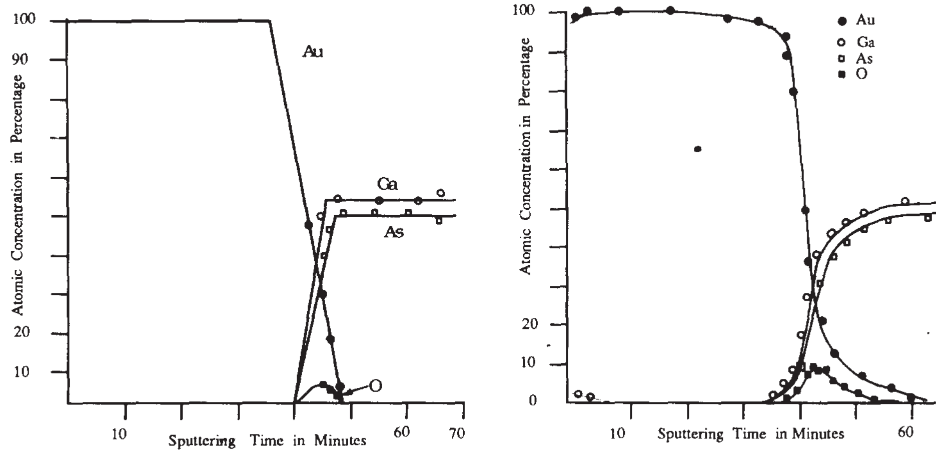

Fig. 1. Auger depth profile of an as-deposited Au–GaAs system.

Fig. 2. Auger depth profile of an Au–GaAs contact annealed at 450 °C for 5 min.

3. ANALYSIS AND DISCUSSION

Assuming grain boundary diffusion, the gallium concentration in gold grains is determined applying Whipple's grain boundary diffusion theory[7].

$$2aD_{\rm B} = \left\{\frac{\partial(\ln C)}{\partial(x^{6/5})}\right\}^{-5/3} \left(\frac{4D_{\rm L}}{t}\right)^{1/2} (0.78)^{5/3} \tag{1}$$

Here $D_{\rm B}$ and $D_{\rm L}$ are grain boundary and lattice diffusivities respectively; $2a$ is the grain boundary width; C is the gallium concentration at a depth x from Au/GaAs interface; t is the anneal time. If $D_{\rm L}$ and t are known in eqn. (1), $2aD_{\rm B}$ can be determined by calculating the slope from the linear region of the $\ln C$ *vs.* $x^{6/5}$ plot.

Such a plot for three samples annealed at three different temperatures, *i.e.* 300 °C, 400 °C and 450 °C are shown in Fig. 3. Other samples had minute amounts of copper which enhanced diffusion of the constituents and the data was not reliable in those samples.

Since both D_B and D_L are unknown, the ratio $2aD_B/D_L^{1/2}$ is determined and given in Table I. In order to calculate D_L, an approximate solution of grain boundary diffusion obtained by Fisher is used[8].

$$\frac{C}{C_0} = \exp\left\{-\left(\frac{4\pi}{t}\right)^{1/4}\left(\frac{2aD_b}{D_L}\right)^{1/2} x\right\} \operatorname{erfC}\frac{(y-a)}{2(D_L t)^{1/2}} \tag{2}$$

Here y is the horizontal axis parallel with the sample surface. To estimate D_L from eqn. (2), we chose the largest x (x_m) where the Auger signal is a minimum. Since gold grains grow bigger for higher anneal temperatures[9,10], $y-a$ is set for different values as shown in Table II. Thus, D_L and D_B are determined and given in Table II. The value of D_B reported here is almost three orders of magnitude higher than that reported by Gupta *et al.*[3] The deposition method of the gold film and the technique of estimation of D_L are different in each case. Based on the calculated values of D_B and D_L an Arrhenius plot is made as shown in Fig. 4 to obtain the temperature dependence of D_L and D_B. The results are

$$D_L = 6.5 \times 10^{-13} \exp(-0.33\text{eV}/kT)\,\text{cm}^2\,\text{s}^{-1}$$
$$D_B = 3.5 \times 10^{-9} \exp(-0.21\text{eV}/kT)\,\text{cm}^2\,\text{s}^{-1}$$

The values of D_0 and E_a obtained here for grain boundary diffusion (D_B) are comparable with the values for gallium diffusion in Ni/AuGe layers ($E_a = 0.1$ eV, $D_0 = 2 \times 10^{-12}\,\text{cm}^2\,\text{s}^{-1}$) estimated by Robinson[11], and close to the value of $D_0 = 4.5 \times 10^{-8}\,\text{cm}^2\,\text{s}^{-1}$ reported by Gupta *et al.*[3].

The values of D_L and D_B for gallium diffusion in gold reported here are also not too far off the reported values of D_L and D_B based on the grain boundary diffusion of metals such as platinum, chromium and silver in gold films[12,13].

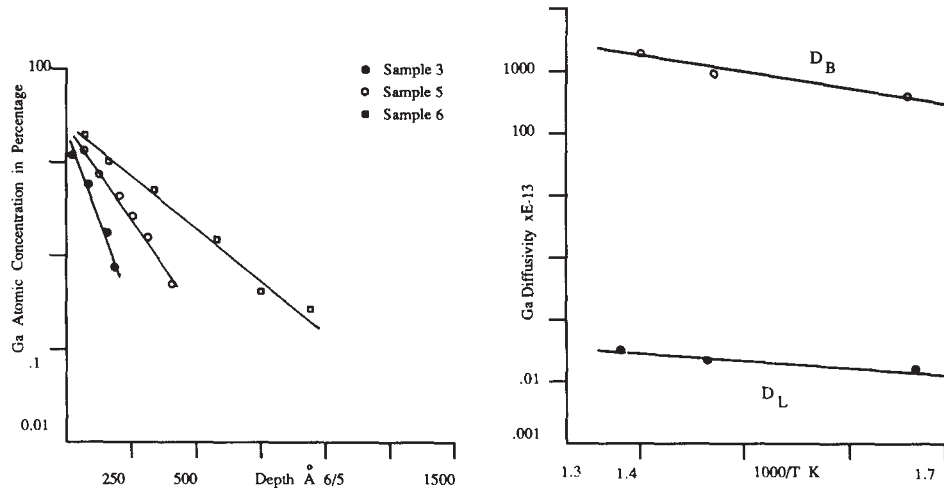

Fig. 3. Gallium diffusion in gold based on grain boundary diffusion equation.

Fig. 4. Arrhenius plot of gallium diffusivity in gold layer.

TABLE I
GALLIUM DIFFUSIVITY CALCULATIONS

Sample	Annealing temperature T (°C)	Annealing time t (s)	(Slope)$^{-5/3}$ (cm^2)	$2aD_B/D_L^{1/2}$ (cm^2 s^{-1})
3	300	300	1.14×10^{-9}	8.73×10^{-11}
5	400	300	1.20×10^{-9}	9.10×10^{-11}
6	450	300	1.44×10^{-9}	10.98×10^{-11}

TABLE II
GALLIUM DIFFUSIVITY IN GOLD LAYER ($2a = 0.5$ nm)

Sample	x_m (nm)	C (%)	y–a (nm)	D_L (cm^2 s^{-1})	D_B (cm^2 s^{-1})
3	11.51	0.006	20	0.89×10^{-15}	5.2×10^{-11}
5	14.43	0.025	25	2.20×10^{-15}	8.5×10^{-11}
6	40.88	0.007	30	3.60×10^{-15}	13.1×10^{-11}

The concentration of gold as a function of distance, in GaAs, as seen in Figs. 1 and 2 shows two distinct regions; one with a sharp initial drop at the interface and the other with a continuous decrease in the interior of the GaAs substrates. This is believed to be the result of two factors[14,15]: (i) the presence of a high concentration of vacancies that act as "traps" of gold atoms on the GaAs surface and (ii) diffusion of gold along interstices. Thus, for short annealing durations, the gold concentration of the initial portion is $C\exp(-x K^{1/2}/D^{1/2})$ and the gold concentration in the interior of the GaAs substrate is $C = C_0 \mathrm{erf}C\{x/2(Dt_a)^{1/2}\}$. Here C is the atomic concentration, x is the diffusion length, K is the probability of capture of a gold atom by a trap and t_a is the annealing time. Hence, the diffusivity of gold in GaAs may be determined and is given in Table III. The data in samples 2 and 4 may have been enhanced because of the presence of copper in these samples. The data for samples 6 and 7 can be expressed as

$$D_{Au} = 3.12 \times 10^{-3} \exp(-1.59\,\mathrm{eV}/kT)\,\mathrm{cm^2\,s^{-1}}$$

These values are close to the values for silver diffusion in GaAs ($E = 1.5$ eV, $D_0 = 2.5 \times 10^{-3}$ cm^2 s^{-1})[15].

TABLE III
GOLD DIFFUSIVITY IN GALLIUM SUBSTRATES

Sample	Annealing temperature (°C)	Slope of initial drop (nm^{-1})	K/D (cm^{-2})	D in interior (cm^2 s^{-1})
2	250	0.069	4.8×10^{11}	1.0×10^{-13}
4	350	0.081	6.5×10^{11}	4.1×10^{-14}
6	450	0.079	6.2×10^{11}	2.8×10^{-14}
7	500	0.072	5.2×10^{11}	1.4×10^{-13}

4. CONCLUSIONS

The grain boundary diffusion mechanism applied to the diffusion of gallium into gold in Au/GaAs contacts provides useful information on the diffusion parameters. The diffusion parameters are determined on the basis of concentrations obtained from sputter Auger depth profiles.

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