INTERDIFFUSION STUDY IN SYSTEMS OF Ta-Si

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Transition metal silicides possess excellent mechanical properties, high strengths, high melting points, high creep resistance at elevated temperature, and good resistance to oxidation, which has attracted the extensive attention of many researchers. The main reason for this is the silicides have high-temperature stability and have low resistivity [1]. They can be used as Schottky barriers and Ohmic contacts in integrated-circuit technology. Recently, interest in silicides has increased considerably because of their potential usefulness as low-resistivity contacts, gate and interconnection metallization in silicon-integrated circuits. The evolution of very large scale integration (VLSI) has necessitated a further study in transition metal silicides, such as their thermodynamic, electrical, and mechanical properties, and their stability at high temperatures.

Among these silicides, tantalum silicide is important in the microelectronics industry for the use as interconnects and contacts because of thermal stability and low contact resistance [2]. This is produced by reaction-diffusion at the metal-silicon interface in the solid state. Tantalum silicide ($TaSi_2$) is the potential high temperature material and micro-electronic material. $TaSi_2$ is mainly used as a high-temperature reinforcing material to improve the oxidation resistance, thermal shock resistance, compactness. As so far, the structural stability, mechanical, thermodynamic properties and high temperature oxidation of $TaSi_2$ silicide have also been investigated by experimental and theoretical methods. Experimental and theoretical results indicate that $TaSi_2$ silicide exhibit the brittle behavior [3].

The authors [4] show the phase diagram of Ta-Si, as shown in figure 1. It can be seen in the Ta-Si phase diagram that there are four phases are present and therefore all these phases are expected to grow in a Ta/Si diffusion couple.

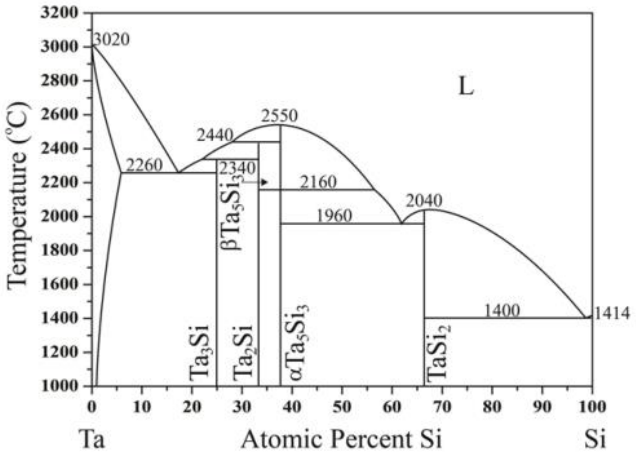

Fig.1. Ta-Si phase diagram

The rate constants of the second kind are useful parameters to describe the diffusion-controlled growth of compounds in binary metal-silicon diffusion couples. The rate constant of the second kind is directly related to the diffusion properties and to the thermodynamic stability of the given phase. The interdiffusion coefficients in Ta_5Si_3 and $TaSi_2$ were obtained from the layer growth kinetics measured on Ta-Si diffusion couples at 1250-1350°C. The activation energies for diffusion, ~450 kJ mol^{-1} for Ta_5Si_3 and ~560 kJ mol^{-1} for $TaSi_2$, are quite high if compared to those usually found for transition-metal silicides. Integrated diffusion coefficients in the $TaSi_2$ and Ta_5Si_3 phases are shown in Figure 2-3.

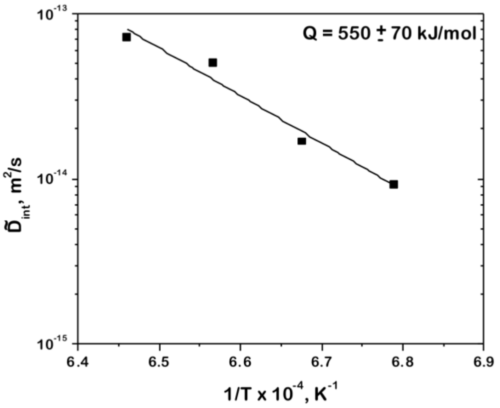

Fig. 2. Integrated diffusion coefficient in the $TaSi_2$ phase.

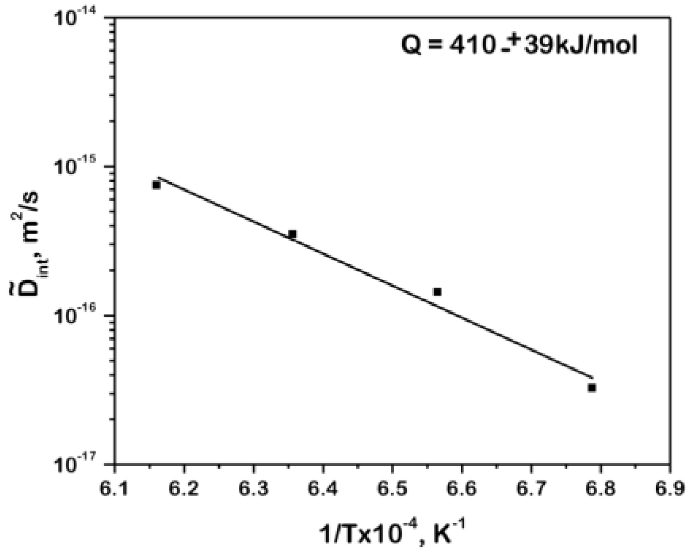

Fig.3. Integrated diffusion coefficient in the Ta_5Si_3 phase.

The interdiffusion coefficients as obtained above represent average values through the given compound layer because of the existence of a chemical potential gradient. In the case of nonisotropic crystals, like Ta_5Si_3 and $TaSi_2$, the diffusion coefficient also depends on the crystallographic direction. If the grains have a random orientation, the diffusion coefficient obtained for a polycrystalline layer represents an average value. However, in the case of $TaSi_2$, the development of elongated columnar grains can reflect a strong texture of the layer and, therefore, the tendency to grow in the direction in which diffusion is faster. This may lead to differences between the interdiffusion coefficient obtained from growth kinetics and the tracer diffusion coefficient measured on polycrystalline materials. In turn, these differences can result in different values of the activation energy.

References

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