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Reliability of Epitaxial Nickel Disilicide Thin Film

Cheng-Lun Hsin[1] and Sheng-Wei Lee[2]

[1]Department of Electrical Engineering, National Central University
[2]Institute of Materials Science and Engineering, National Central University

No.300, Chongda Rd., Chongli district, Taoyuan city, Taiwan, 32001
Phone: +886-3-422-7151 ext 34520 E-mail: clhsin@ee.ncu.edu.tw

Abstract

In this report, epi-$NiSi_2$ with an atomically flat interface was formed with a controlled process and its structure was examined by electron microscopy. The interface between the epitaxial silicide and Si substrate is atomically flat. The fabrication process is compatible with Si-based CMOS technology. The structural advantage of the epitaxial silicide can eliminate the disadvantage of conventional NiSi by reducing the barrier height and junction leakage. The reliability, which was investigated under different temperatures and current densities to understand its electronic characteristics, was 1.5 times better than that of the conventional polycrystalline counterpart. Black's equation and the measured mean-time-to-failure (MTTF) were used to obtain the reliability characteristics of epitaxial and poly-$NiSi_2$. Our results provide evidence that epitaxial $NiSi_2$ is a promising contact material for future electronics.

1. Introduction

The feature size of metal-oxide-semiconductor field-effect transistors (MOSFET) has now been scaled down below twenty nanometers[1]. The difficulties in pursuing next generation technologies to meet Moore's law have dramatically increased for research and development[2]. For the MOSFET, metal silicides have been used as contact materials for many decades[3]. However, two of the most confronting issues among these technical barriers in the metal silicides are the contact and series resistance, and traditional self-aligned silicidation processes has faced the limitation on low sheet resistance for future applications due to the decrease of the source/drain contact area[4]. Since the 90-nm technology node, NiSi has been the material most extensively used in source/drain contacts, owing to its low consumption of Si, small narrow line-width effect, and low formation temperature. But the poor thermal stability of the nanoscaled thin film has become a serious issue in recent years[5]. At high temperatures, NiSi over ten-nanometers in thickness would agglomerate to become nanodots easily, resulting in the narrowing of the process window[6]. Besides, the rough interface between nano-scaled NiSi and Si would cause the increase of leakage current[7], and the differences in thermal expansion coefficient and crystal structure between NiSi and Si is large enough to induce dislocations during the formation process [8]. Additionally, the series resistance of contemporary NiSi is still too high for MOSFET in next generation[9]. Recently, initial studies on ultra-thin epitaxial metal silicides have been carried out. The growth of epitaxial $NiSi_2$ (epi-$NiSi_2$) by a Ni thin film under the critical thickness (about 4.2 nm) deposited on a Si wafer has been observed at low temperatures without other Ni-rich intermediate phases. Below this critical value, the surface energy and the reduction of the interfacial energy caused by the small thickness played an important role in the heat of formation, making $NiSi_2$ become energetically favorable and epitaxial aligned. In these previous studies, epi-$NiSi_2$ thin films less than 10 nm in thickness with an atomically flat interface were grown on the surface. Moreover, the specific contact resistivity and Schottky barrier height of epi-$NiSi_2$ is lower than that of NiSi on both As- and B-doped Si-on-insulator and strained-Si-on-insulator. This structural and electrical advantage makes ultra-thin epi-$NiSi_2$ to be a potential candidate to replace NiSi as the contact material in the future.

2. General Instructions

The thin Ni film was deposited on the Si substrates. After dipping the samples in sulfuric acid solution, a 5-nm-thick Ni/Si intermixed layer was exposed, and this amorphous structure was formed due to the high-power sputtering. The presence of this layer made the growth of the ultra-thin epi-$NiSi_2$ possible after RTA (Fig. 1a). It is believed that the Ni/Si ratio of the intermixed layer could be adjusted by altering the sputtering process parameters, and the thickness of the epilayer could be controlled. Besides, this method is much reliable and repeatable than controlling the as-deposited thickness by evaporation. To compare the typical thickness ratio of the resulting silicide per nm of Ni (3.63) in previous reports, and the thicknesses of the intermixed layer and epi-$NiSi_2$ layer in this study, we believe that stoichiometric Ni was sputtered into the intermixed layer, making the composition ratio of the intermixed layer close to the stoichiometric ratio of the compound, based on the law of mass conservation. This may result in a low formation temperature as a result of a lowered Gibbs free energy. In this case, the intermixing layer will tend to form $NiSi_2$ at low temperatures, allowing it to nucleate epitaxially[12]. The epitaxial relationship between the epi-$NiSi_2$ and Si substrate was $NiSi_2$(001)[110]||Si(001)[110], which was also confirmed by XRD analysis, as shown in Fig. 1b. The spectrum shows two distinct XRD peaks. The crystal structure and lattice constant of $NiSi_2$ is very similar to Si,

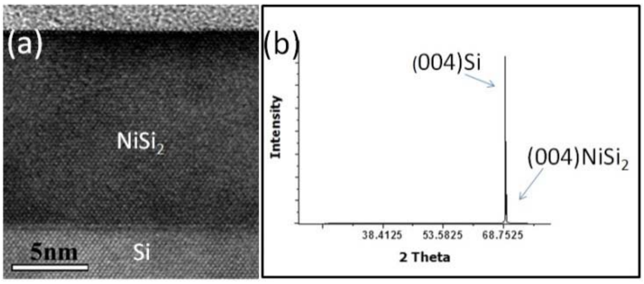

Figure 1. (a) Cross-sectional TEM images of $NiSi_2$ film after RTA process, and (b) XRD spectrum of the epi-$NiSi_2$ on the (001)Si substrate, highlighted two distinct diffraction peaks of Si (on the left) and$NiSi_2$ (on the right).

which is cubic CaF_2-type and 0.541 nm with less than 0.4% mismatch, respectively. The XRD spectrum of our sample only contains two peaks. The left peak (labeled 69.138) is belonging to the (004)Si, while the right one (labeled 69.346) is of (004)$NiSi_2$. This result confirmed the epitaxy of $NiSi_2$ and the Si substrate in large area.

The measurements were carried out at different current densities (5 MA/cm^2 and 10 MA/cm^2) and temperatures (200, 250, and 300 °C). A 10% increase in resistance was defined as the failure criterion, and the failure time was recorded. The reliability results (cumulative distribution versus time) at different temperatures and current densities are summarized in Fig. 2(a) and (b), respectively. It is obvious that the failure time increased at lower temperatures and current densities and that the mean-time-to-failure (MTTF) of epi-$NiSi_2$ was higher than that of poly-$NiSi_2$, proving that epi-$NiSi_2$ is more robust than poly-$NiSi_2$. Black's equation was used to calculate the electromigration-mode characteristics and is given in the following form

$$MTF=Aj^{-n}\exp(E_a/kT), \quad (1)$$

where E_a is the activation energy, j is the current density, n is the current density exponent, and A is a constant. These parameters are listed in Table 1. In addition, the MTTF of epi- and poly-$NiSi_2$ under the condition of room temperature and 2 MA/cm^2 in current density were extracted to clarify the performance of each silicide. The results demonstrated that the reliability of the epitaxial structure was 1.5 times better than that of the conventional polycrystalline ones. Considering the variation in resistance, we calculated confidence intervals (CI) at 95% for each MTTF to investigate the failure mode. The value of the confidence margin is defined as the average of time to failure ± two standard deviations (σ). A single failure mode could be ascertained because all the experimental data remained within these confidence margins. The smaller E_a and n indicated that epi-$NiSi_2$ was less temperature- and current-density-dependent than poly-$NiSi_2$.

3. Conclusions

In this report, epi-$NiSi_2$ with an atomically flat interface was formed with a controlled process and its structure was examined by electron microscopy. The interface between the epitaxial silicide and Si substrate is atomically flat. The fabrication process is compatible with Si-based CMOS technology. The structural advantage of the epitaxial silicide can eliminate the disadvantage of conventional NiSi by reducing the barrier height and junction leakage. Our results provide evidence that epitaxial $NiSi_2$ is a promising contact material for future electronics.

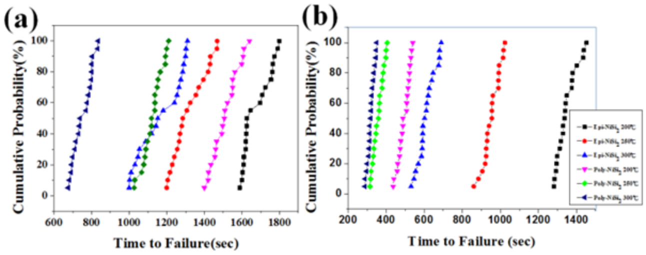

Figure 2. Cumulative distribution versus time to failure at (a) 5 MA/cm^2 and (b) 10 MA/cm^2.

	Conditions (℃)/(MA/cm²)	MTTF (sec)	CI95%	E_a (eV)	n	MTTF at 27℃ and 2 MA/cm² (year)
Epi-$NiSi_2$	200/5	1626	1382~1774	0.62 ±0.08	1.7 ±0.03	7.32 ±0.54
	250/5	1285	1157~1527			
	300/5	1152	1029~1389			
	200/10	1339	1245~1453			
	250/10	956	866~1042			
	300/10	602	522~702			
poly-$NiSi_2$	200/5	1506	1376~1648	0.71 ±0.11	2.1 ±0.05	4.95 ±0.69
	250/5	1119	1020~1228			
	300/5	738	651~855			
	200/10	488	403~619			
	250/10	359	270~441			
	300/10	317	258~394			

Table 1. The measurement condition, MTTF, CI 95%, E_a, n and MTTF at 27 °C and 2 MA/cm^2 of epi-$NiSi_2$ and poly-$NiSi_2$.

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