Structure determination of the ordered $(\sqrt{3} \times \sqrt{3})R30^\circ$ phase of Ni_2Si and Ni_2Ge surface alloys on $\text{Ni}(111)$ via low-energy electron diffraction

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Abstract:

The $(\sqrt{3} \times \sqrt{3})R30^\circ$ structures of 2-D nickel silicide and nickel germanide surface alloys on $\text{Ni}(111)$ were investigated using quantitative low-energy electron diffraction analysis. The unit cells of the determined silicide and germanide structures contain two Ni atoms and one Si or Ge atom, corresponding to the chemical compositions Ni_2Si and Ni_2Ge , respectively. Both the Si and Ge atoms adopt substitutional face-centered cubic hollow sites to sit on the $\text{Ni}(111)$ substrates, and the alloy surfaces exhibit a slight corrugation. The Ni-Si and Ni-Ge distances were 2.44 and 2.56 Å, respectively, and corresponded well to their respective empirical radii. It was also found that the Ni atoms in the second and third layers moved toward the Si or Ge atom sites from their bulk crystal positions. These results indicate rather strong interactions of the Ni atoms with both the Si and Ge atoms at the surface, leading to trapping of the Si and Ge atoms at the substitutional sites without diffusion into the bulk.

Keywords: Low energy electron diffraction (LEED); Surface structure determination; $\text{Ni}(111)$; Si; Ge

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1. Introduction

Understanding of ultra-thin film formation has progressed significantly over the last several decades. Most studies on ultra-thin film technology have primarily focused on the growth of two-dimensional (2-D) layers due to their different properties compared with those of bulk materials. Surface alloys formed only in confined regions on the surfaces of thin films, possibly during the dissolution process, may have new physical and chemical properties due to their thinness.

The crystallographic structural differences are significant for metal on semiconductor (M/S) and semiconductor on metal (S/M) systems with respect to their chemical binding (metallic versus covalent and vice versa). In such M/S and S/M materials, strong structural effects, i.e., the formation of ordered and amorphous alloys, has been observed. The effects of surface alloy formation by metals on metals on the magnetism of materials and their chemical processes have been well investigated [1-6]. In addition, surface alloys formed by metals on semiconductors have been widely studied in order to gain a greater understanding of Schottky barrier formation [7-9]. However, there have been very few reports on S/M systems.

Typical examples of M/S systems include Ag/Si, Au/Ge and Ni/Si [10-12]. Using low-energy electron diffraction (LEED), low-energy electron microscopy (LEEM), and scanning tunneling microscopy (STM), the conditions for nucleation and growth of 2-D phases at Ni/Si interfaces have been extensively investigated [13-15]. The formation of $(\sqrt{3} \times \sqrt{3})R30^\circ$, $(\sqrt{19} \times \sqrt{19})R23.4^\circ$, and (1×1) – ring cluster phases of 2-D surface layers have been studied during the reaction of an ultra-thin film of Ni on a Si(111) substrate [12, 16-19]. The nucleation of a Ni₂Ge thin film on Ge(111) has also been reported [20].

Typical examples of S/M systems include Si/Ag, Ge/Ag, and Si/Ni [21-24]. Recently the S/M systems have drawn attention in nanophysics to understand the surface structure and reaction kinetics at the interface. Our group have reported the Ag-Si 2-D surface alloy formation on Ag(111) substrate at high temperature [21]. Similarly Oughaddou et al. reported an Ag₂Ge surface alloy formation on Ag(111) substrate [22] and the electronic properties of the Ag₂Ge surface alloy have been reported by Golias et al. using angle-resolved photoelectron spectroscopy and DFT calculations [24]. Bulk phase diagrams suggest that there is the possibility for Si or Ge to diffuse into bulk Ni, which is not the case for the reverse system [25]. Lalmi et al. investigated a Si/Ni system to determine the effect of the nonequivalence of Ni/Si and Si/Ni deposition sequences on the initial stages of Schottky barrier

formation [23]. They reported the formation of a 2-D nickel silicide with one-third monolayer (ML) Si-coverage as a $(\sqrt{3} \times \sqrt{3})R30^\circ$ phase [23], but did not do a detailed structural analysis. To the best of our knowledge, there are no available reports concerning Ge on Ni(111).

In the present study, Si and Ge adsorption on Ni(111) were investigated after annealing at 850 and 800 K, respectively. Surface structures of the ordered $(\sqrt{3} \times \sqrt{3})R30^\circ$ phase of the formed 2-D nickel silicide and germanide were determined to have the chemical compositions Ni_2Si and Ni_2Ge , respectively, using quantitative LEED analysis.

2. Experimental

Experiments were performed in an ultrahigh-vacuum (UHV) chamber equipped with a four-grid LEED and Auger electron spectroscopy (AES) analysis system in which the base pressure was 1×10^{-8} Pa. A Ni(111) substrate was cleaned using several cycles of Ar-ion sputtering (1.0 kV, 1 μA , 15 min) and subsequent annealing at 1050 K for 7 min until a sharp $p(1 \times 1)$ LEED pattern was obtained. The deposition of Si or Ge was performed by directly heating a piece of Si or Ge wafer. The temperature of the Ni(111) substrate was monitored using a thermal spot sensor (FTZ6, Japan Sensor Corporation) that was calibrated using a K-type thermocouple.

The LEED optics was placed in the UHV chamber in order to characterize the structural evolution. A digital charge-coupled device camera with a computer-controlled data acquisition system was deployed to measure the LEED spot intensities [26]. The $I(E)$ curves of the LEED spots were obtained within the incident energy range 100–350 eV at 150 K for the structural analysis. The Barbieri-Van Hove symmetrized automated tensor LEED package was used to determine the atomic positions [27], and an imaginary part of the inner potential (V_{oi}) of -5.0 eV was used for damping of the incident electrons. The automated search algorithm was guided by Pendry's reliability factor (R_p) [27, 28]. The best agreement between the experimental and theoretical $I(E)$ curves was determined by minimizing the R_p value. Errors in the structural parameters were estimated using the variance of R_p , $\Delta R = R_p \left(\frac{8|V_{oi}|}{\Delta E} \right)^{1/2}$ [28].

The derivative mode was used to obtain the Auger spectra, and a computer system was deployed to collect the data and determine the peak-to-peak heights of the Auger signals of the elements close to the surface.

3. Results and discussion

Figure 1 shows the obtained LEED patterns for Si and Ge adsorption on Ni(111). First, the Ni(111) substrate was cleaned by sputtering and subsequent annealing, as mentioned in the experimental section. Next, Si was deposited on the Ni(111) substrate for 8 min at room temperature (RT), and the LEED pattern was observed without any subsequent annealing. In this case, no change in the LEED pattern was detected except the (1×1) LEED pattern for Si with a high background for the clean Ni(111). The Ni(111) sample was then annealed by gradually heating from RT to 920 K. No change in the (1×1) pattern was observed up to 600 K. After annealing at 650 K, however, a faint $(\sqrt{3} \times \sqrt{3})R30^\circ$ LEED pattern was detected, which was clear at an annealing temperature of 850 K. The second and third steps were then repeated using Si deposition times of 2–30 min with an equal step of 2 min (on clean Ni(111)). No phase change was observed even after annealing for Si deposition times up to 6 min. On the other hand, as the time for Si deposition on Ni(111) was gradually increased from 7 to 30 min, the $(\sqrt{3} \times \sqrt{3})R30^\circ$ LEED pattern was observed after annealing (third step). The sharpest $(\sqrt{3} \times \sqrt{3})R30^\circ$ LEED pattern for quantitative analysis was obtained at a Si deposition time of 12 min with annealing at 850 K, and is shown in Fig. 1 (a). Next, the deposition method was changed while all of the other conditions remained the same, and Si was deposited for 2 to 30 min. In this deposition method, the Si deposition time was not only increased chronologically, rather cleaning the sample via sputtering, Si deposition, and annealing were done all together for every incremental steps of 2 min for Si deposition. Once again, only the $(\sqrt{3} \times \sqrt{3})R30^\circ$ LEED pattern was obtained for Si deposition times of 6 to 12 min. However, at Si deposition times of 14 to 16 min, a mixed phase LEED pattern for $(\sqrt{3} \times \sqrt{3})R30^\circ$ and (2×2) phases was obtained, whereas at Si deposition times of 20 to 30 min, only the (2×2) LEED pattern was observed. The Si deposition rate was about 0.028 ML/min, where the monolayer (ML) is defined as one Si atom adsorption onto one Ni atom.

For the experiments with Ge, similar steps were followed. As was observed for Si deposition, no phase transition except the (1×1) phase for Ge deposition on Ni(111) was observed up to 600 K. A very faint

$(\sqrt{3} \times \sqrt{3})R30^\circ$ phase was obtained after 45 min of Ge deposition followed by annealing at 650 K that sharpened with increasing deposition time. The sharpest $(\sqrt{3} \times \sqrt{3})R30^\circ$ LEED pattern for quantitative analysis was obtained after 70 min of Ge deposition followed by annealing at 800 K, and is shown in Fig. 1 (b). Notably, no phase transitions other than the $(\sqrt{3} \times \sqrt{3})R30^\circ$ phase were observed for Ge deposition up to 140 min using both deposition methods described in the previous section. However, when the annealing temperature was greater than 850 K, the (1×1) phase with a high background was obtained instead of the $(\sqrt{3} \times \sqrt{3})R30^\circ$ phase. The Ge deposition rate was about 0.005 ML/min.

The Si-coverage on Ni(111) was determined using AES. Figure 2 shows the AES intensity versus energy curves for the clean Ni(111) substrate and the $(\sqrt{3} \times \sqrt{3})R30^\circ$ phase of Si on Ni(111). The peak-to-peak height ratio (PHR) for Si (92 eV) to Ni (61 eV) was determined to be ~ 0.23 for the $(\sqrt{3} \times \sqrt{3})R30^\circ$ phase, which is similar to the value reported by Lalmi et al. [23]. The Si-coverage was reported to be $1/3$ ML. The PHR for Ge to Ni could not be determined, however, because the AES peaks for Ge (52 eV) and Ni (61 eV) are very close.

To determine the surface structures of the $(\sqrt{3} \times \sqrt{3})R30^\circ$ phases of Si and Ge on Ni(111), two sets of experimental $I(E)$ curves were obtained for the various LEED spots from the stored LEED patterns, and twelve models, as depicted in Fig. 3, were examined for both. The first layers of models 1–3, 6, 9, and 12 contain only Si (or Ge) atoms; on the other hand, the first layers of models 4, 5, 7, 8, 10, and 11 are composite layers of Si (or Ge) and Ni. The remaining lower layers in all of the models consisted only of Ni atoms. All of the models have $p31m$ symmetry, and the atomic positions of the Si (or Ge) and the positions of the composite surface layers and adjacent two lower Ni layers were adjusted to optimize the R_p values. The Ni atoms below the third layer were maintained in the bulk position. The top sites of the substrate Ni atoms were treated as adsorption sites for Si (or Ge) for models 1 and 4–6, whereas the FCC and hexagonal close packing hollow sites were considered to be adsorption sites for models 2 and 7–9 and 3 and 10–12, respectively. The models 1–3 have only one Si (or Ge) atom, whereas models 4, 7, and 10 consist of one Si (or Ge) and two Ni atoms, models 5, 8, and 11 consist of two Si (or Ge) and one Ni atoms, and models 6, 9, and 12 consist of only three Si (or Ge) atoms in the unit cells of their respective topmost composite layers. Although models 6, 9 and 12 apparently look like the (1×1) structure, due to the height difference in the Si (or Ge) atoms in the topmost layer, they are actually $(\sqrt{3} \times \sqrt{3})R30^\circ$

surface structures. The R_p values obtained after optimization of the models for Si and Ge adsorption are listed in Table 1.

For Si adsorption on Ni(111), the R_p values for models 7–9 were less than 0.3, while those for the other models were greater than 0.3, and thus these other models (1–6, 10–12) were disregarded. Model 7 is clearly the best given that it has the lowest R_p value (0.05) of the three remaining models (model 8 = 0.20 and model 9 = 0.22). Further optimization of model 7 was thus performed by adjusting the thermal vibrations (Debye temperatures) for Si and Ni in the topmost layers. The fitted Debye temperatures were 630 and 300 K, respectively. For Ge on Ni(111), model 7 was the best-fit model with $R_p = 0.07$, while the R_p values for all of the other models were greater than 0.3 and thus disregarded. The fitted Debye temperatures for the Ge and Ni atoms in the topmost layers were 300 and 300 K, respectively. A detailed illustration and the structural parameters for model 7 for Si on Ni(111) are shown in Fig. 4 (a) and (b) and Table 2, respectively, and those for Ge on Ni(111) are shown in Fig. 4 (a) and (c) and Table 3, respectively. A comparison of the experimental and theoretical $I(E)$ curves for model 7 for Si and Ge on Ni(111) are presented in Fig. 5 (a) and (b), respectively. It can be seen in these figures that the agreement between the experimental and theoretical $I(E)$ curves is quite good.

From the detailed models shown in Fig. 4, it can be seen that both of the Si and Ge atoms adopt the substitutional FCC hollow sites to sit on bulk Ni(111), and silicide and germanide 2-D alloys are formed only at the topmost surface layers. In both cases, the interlayer distance between the Ni atoms in the topmost layers and those in the next adjacent layer is nearly the same as that found in bulk Ni (2.03, 2.05, and 2.04 Å for Si on Ni, Ge on Ni, and clean Ni(111), respectively, as determined via quantitative LEED analysis). On the other hand, the interlayer distance between Si and Ni is 1.98 Å, and that between Ge and Ni is 2.13 Å. Thus, the Si-Ni and Ge-Ni interlayer distances are less than and greater than that for Ni-Ni, respectively. In both cases, however, the surface corrugation is likely small.

A similar 2-D surface alloy formed via adoption by Ge of substitutional sites in Ag(111) with a $(\sqrt{3} \times \sqrt{3})R30^\circ$ structure was reported by Oughaddou et al. [22], who described a single Ag_2Ge chemical environment for the $(\sqrt{3} \times \sqrt{3})R30^\circ$ structure as determined using photoemission spectroscopy. In the present study, the surface structure for Ge on Ni(111) was also determined to have a single Ni_2Ge chemical environment. In addition, the atom configuration for the $(\sqrt{3} \times \sqrt{3})R30^\circ$ structure for Ge on Ag(111) determined by Golias et al. [24] using DFT calculations is quite similar to the surface structure model for Ge on Ni(111) determined in the present study. Both Oughaddou et al. and Golias et al.

mentioned that the 2-D surface alloy for Ge on Ag(111) has highly metallic characteristics. Therefore, due to the similarity of the Ag₂Ge and Ni₂Ge surface alloys, it is likely that the Ni₂Ge surface alloy also has metallic characteristics, although determination of its electronic properties is necessary in the future.

Si also forms a surface alloy on Ag(111) at high temperatures, but at low temperatures the Si atoms do not strongly interact with the Ag atoms [21, 29]. Specifically, at 600–650 K, the Si atoms adopt substitutional sites on Ag(111) to form a 2-D surface alloy [21], whereas at 490–560 K they bond to themselves to form silicene on Ag(111) [29, 30]. At low temperatures, the Si atoms do not have sufficient energy to displace the Ag atoms from the substrate layer, and therefore bond to one another to form a homoatomic surface layer; on the other hand, at high temperatures, the Si atoms acquire sufficient energy to substitute the Ag atoms and form a 2-D surface alloy with Ag. Unlike Si on Ag(111), in the present study no homoatomic bonds were detected for Si on Ni(111) at low temperatures, although a surface alloy was formed at high temperatures. It should be noted that a higher temperature (650–850 K) was required for Si substitution of Ni atoms to form the surface alloy in the Si on Ni(111) system compared to that for the Si on Ag(111) system, which is consistent with the fact that Ni-Ni bond dissociation energy is higher than that for Ag-Ag [31].

For Si adsorption on Ni(111), electron transfer between the Si and Ni atoms has been reported at high temperatures [23], which indicates that the Si atoms strongly interact with the Ni atoms. Lalmi et al. also reported that the Si atoms are surrounded by Ni atoms, and the chemical environment for the $(\sqrt{3} \times \sqrt{3})R30^\circ$ structure of Si on Ni(111) is Ni₂Si [23]. It can be seen in Fig. 4 that the Si atoms are surrounded by Ni atoms and adopt substitutional sites on the Ni(111) substrate to give a unit cell with the chemical environment Ni₂Si, which is identical to that proposed by Lalmi et al. These researchers also reported that only slight surface corrugation was observed via STM, which is in agreement with the results obtained in the present study.

The Ni(4)-Si(1) and Ni(4)-Ge(1) distances were determined to be 2.44 and 2.56 Å (Tables 2 and 3), respectively. The Ni(4)-Si(1) bond length is smaller than that of Ni(4)-Ge(1) due to the smaller atomic radius of Si compared to that of Ge. The obtained bond lengths agree very well with the empirical atomic radii for Ni, Si, and Ge (1.35, 1.10, and 1.25 Å, respectively) [32]. The Ni-Si bond length is also consistent with that of the binary alloy Ni₂Si [33]. As a result, the substitutional $(\sqrt{3} \times \sqrt{3})R30^\circ$ structure is stable for these systems. Moreover, small displacements of the Ni atoms were observed for the Ni atoms in the second (3, 4, and 5) and third (6, 7 and 8) layers; these atoms move by 0.018 and

0.027 Å, respectively, toward the Si adsorption sites (the origin of the lateral coordinates) with respect to their positions in the bulk crystal. Similarly, second and third layer Ni atoms are displaced by 0.008 and 0.010 Å toward the Ge sites, respectively, in the Ge of Ni(111) system. These displacement values are very small, but this tendency appears to be meaningful, because the results indicate rather strong interactions between the Ni atoms and both the Si and Ge atoms in the topmost surface layers. It is possible that these interactions lead to trapping of the Si and Ge atoms in the substitutional FCC hollow sites and prevent their diffusion deep into the interior of the bulk Ni crystal.

4. Conclusions

The phase evolution for individual Si and Ge adsorption on Ni(111) was investigated using LEED, and in both cases $(\sqrt{3} \times \sqrt{3})R30^\circ$ phases were observed. The surface structures of these $(\sqrt{3} \times \sqrt{3})R30^\circ$ phases for 2-D nickel silicide and nickel germanide were determined using quantitative LEED $I(E)$ analysis. The Pendry's R-factors for the best-fit models were 0.05 and 0.07 for the nickel silicide and nickel germanide surface alloy structures, respectively. The unit cells of the determined silicide and germanide structures contain two Ni atoms and one Si or Ge atom, respectively, and correspond to the chemical compositions Ni_2Si and Ni_2Ge . In addition, the Ni atoms in the second and third layers were found to have moved from their bulk crystal positions toward the Si and Ge sites. These surface structure determinations will be helpful for investigations of Schottky barriers at semiconductor-metal interfaces.

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Figure and table captions

Fig. 1. Obtained LEED patterns for the $(\sqrt{3} \times \sqrt{3})R30^\circ$ phases for (a) Si adsorption on Ni(111) and (b) Ge adsorption on Ni(111).

Fig. 2. AES spectra of the clean Ni(111) surface (dotted line) and the $(\sqrt{3} \times \sqrt{3})R30^\circ$ phase of Si on Ni(111) (red line).

Fig. 3. Structural models evaluated for the $(\sqrt{3} \times \sqrt{3})R30^\circ$ phase formed following Si or Ge adsorption on Ni(111).

Fig. 4. (a) Top view of the best-fit structural model for Si (or Ge) on Ni(111). The black rhombus corresponds to the $(\sqrt{3} \times \sqrt{3})R30^\circ$ unit cell. (b) and (c) Side views of the best-fit models for Si on Ni(111) and Ge on Ni(111), respectively. The numbers in (b) and (c) correspond to the atoms in Tables 2 and 3, respectively.

Fig. 5. Experimental and theoretical $I(E)$ curves for the best-fit models: (a) Si on Ni(111) and (b) Ge on Ni(111).

Table 1. Pendry's R-factors for the models evaluated for Si and Ge adsorption on Ni(111).

Table 2. Structural parameters obtained for the best fit model for the $(\sqrt{3} \times \sqrt{3})R30^\circ$ phase of Si on Ni(111). The parameters in parentheses correspond to those for the bulk crystal of Ni(111) [32].

Table 3. Structural parameters obtained for the best fit model for the $(\sqrt{3} \times \sqrt{3})R30^\circ$ phase of Ge on Ni(111). The parameters in parentheses correspond to those for a bulk crystal of Ni(111) [32].

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Table 1. Pendry's R-factors for the models evaluated for Si and Ge adsorption on Ni(111).

Model number	R_p for Si on Ni(111)	R_p for Ge on Ni(111)
1	0.42	0.45
2	0.35	0.36
3	0.47	0.48
4	0.57	0.58
5	0.53	0.57
6	0.46	0.52
7	0.05	0.07
8	0.20	0.31
9	0.22	0.30
10	0.53	0.54
11	0.53	0.55
12	0.64	0.63

Table 2. Structural parameters obtained for the best fit model for the $(\sqrt{3} \times \sqrt{3})R30^\circ$ phase of Si on Ni(111). The parameters in parentheses correspond to those for the bulk crystal of Ni(111) [32].

Atom (No.)	$[\bar{1}10]$ (Å)	$[\bar{1}\bar{1}2]$ (Å)	$[111]$ (Å)
Ni (1)	1.246	2.158	-2.034 ± 0.007
Ni (2)	-1.246	2.158	-2.034 ± 0.007
Si (1)	0.000	0.000	-1.982 ± 0.015
Ni (3)	0.000 ± 0.016 (0.000)	1.421 ± 0.016 (1.439)	0.000 ± 0.007 (0.000)
Ni (4)	1.231 ± 0.016 (1.246)	-0.711 ± 0.016 (-0.719)	0.000 ± 0.007 (0.000)
Ni (5)	-1.231 ± 0.016 (-1.246)	-0.711 ± 0.016 (-0.719)	0.000 ± 0.007 (0.000)
Ni (6)	0.000 ± 0.027 (0.000)	-1.411 ± 0.027 (-1.439)	2.038 ± 0.021 (2.035)
Ni (7)	1.222 ± 0.027 (1.246)	0.706 ± 0.027 (0.719)	2.038 ± 0.021 (2.035)
Ni (8)	-1.222 ± 0.027 (-1.246)	0.706 ± 0.027 (0.719)	2.038 ± 0.021 (2.035)

Table 3. Structural parameters obtained for the best fit model for the $(\sqrt{3} \times \sqrt{3})R30^\circ$ phase of Ge on Ni(111). The parameters in parentheses correspond to those for a bulk crystal of Ni(111) [32].

Atom (No.)	$[\bar{1}10]$ (Å)	$[\bar{1}\bar{1}2]$ (Å)	$[111]$ (Å)
Ge (1)	0	0	-2.125 ± 0.014
Ni (1)	1.246	2.158	-2.047 ± 0.009
Ni (2)	-1.246	2.158	-2.047 ± 0.010
Ni (3)	0.000 ± 0.014 (0.000)	1.431 ± 0.014 (1.439)	0.000 ± 0.010 (0.000)
Ni (4)	1.239 ± 0.014 (1.246)	-0.716 ± 0.014 (-0.719)	0.000 ± 0.010 (0.000)
Ni (5)	-1.239 ± 0.014 (-1.246)	-0.716 ± 0.014 (-0.719)	0.000 ± 0.010 (0.000)
Ni (6)	0.000 ± 0.021 (0.000)	-1.429 ± 0.021 (-1.439)	2.037 ± 0.021 (2.035)
Ni (7)	1.237 ± 0.021 (1.246)	0.714 ± 0.021 (0.719)	2.037 ± 0.021 (2.035)
Ni (8)	-1.237 ± 0.021 (-1.246)	0.714 ± 0.021 (0.719)	2.037 ± 0.021 (2.035)