Microstructural characterization of ordered nickel silicide structures grown on (111) nickel silicide films

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The formation processes of epitaxial nickel silicides, resulting from the interaction of nickel silicide films (10 nm–100 nm) on (111) silicon (Si) substrates after furnace annealing, have been studied using transmission electron microscopy (TEM) and x-ray diffraction (XRD) techniques. The formation of type-A epitaxial grains (i.e., grown with the same orientation of the underlying Si substrate) and type-B epitaxial grains (i.e., rotated by 180° around the surface normal) in "thick" epitaxial films (i.e., greater than 35 nm) is proposed to be linked to the formation of a fluorite-based CuPt ($L1_1$)-like NiSi phase. This phase is found to be a metastable phase and is believed to be a transitional phase toward the formation of the equilibrium $NiSi_2$ phase in both type-A and type-B orientations. In addition, we have found that a fluorite-based CuPt-like NiSi may even coexist with a fluorite-based CuAu I-like structure. The interrelationship between these two structures is discussed in the context of a displacive transformation process in fcc structures as originally proposed by Hansson and Barnes [Acta Metall. **12**, 315 (1964)] and Pashley *et al.* [Philos. Mag. **19**, 83 (1969)].

I. INTRODUCTION

Recent studies into the formation mechanisms of epitaxial nickel silicides on (111)Si substrates have shed light onto the unique phase transformation processes that occur. Bennett *et al.* have shown that crystalline Ni and $\delta-Ni_2Si$ phases (orthorhombic, space group: *Pnma*) existing as intermediate structures during the formation of $NiSi_2$ in "thin" epitaxial layers (~8.5 nm).[1] It is concluded that the two phases are not directly involved in the formation of the equilibrium phase, $NiSi_2$. Gibson *et al.* have shown in Ultra-High Vacuum (UHV) studies that a transition phase, $\theta-Ni_2Si$ (hexagonal, space group *hP6*), is coupled to the formation of "ultrathin" (i.e., less than 3.5 nm thick) type-A $NiSi_2$.[2] In their study, dark-field TEM images taken in the early stages of epitaxial formation show areas of $\theta-Ni_2Si$ existing within the TEM sample. Upon annealing, type-A $NiSi_2$ is found to reside in the same location as that of $\theta-Ni_2Si$. Type-B $NiSi_2$ is observed to form in an extremely rapid manner and encompasses much of the TEM sample. In a more recent study of "thick" (~350 nm) nickel silicide films grown on (111)Si substrates, Ho *et al.* have shown that ordered metastable epitaxial nickel silicide phases exist prior to the formation of the $NiSi_2$ phase.[3] Two metastable phases that are found in significant amounts in epitaxial grains are a CaF_2-based CuAu I ($L1_0$)-like structure and a CaF_2-based CuPt ($L1_1$-like) structure. It is proposed that the formation of the CuPt-like structure is coupled to the formation of type-A and type-B orientations found in (111) epitaxial nickel silicide films. The authors presented an overview as to the possible unit cell structures of these metastable phases based on TEM electron diffraction analysis. However, little evidence is given concerning: (i) the link between the CuPt-like phase to the two orientations of $NiSi_2$, and (ii) to the transformation process of the $L1_0$-like structure into the $L1_1$-like structure. In the present paper, the authors provide additional evidence confirming the existence of the fluorite-based CuPt-like structure in epitaxial films 35 nm–350 nm thick. In addition, a possible transformation mechanism of the CuAu I-like structure into the CuPt-like structure is presented.

II. EXPERIMENTAL

Nickel thin films (10 nm–100 nm) were sputter-deposited onto (111)Si wafers. The thin film-Si composites were then annealed in a three-zone furnace sealed at both ends under a continuous flow of forming gas (90% N_2–10% H_2) or under a 98% Ar–2% H_2 mixture (purity of Ar > 5–9's). The temperature range of 650 °C–825 °C was chosen in our experiments. A

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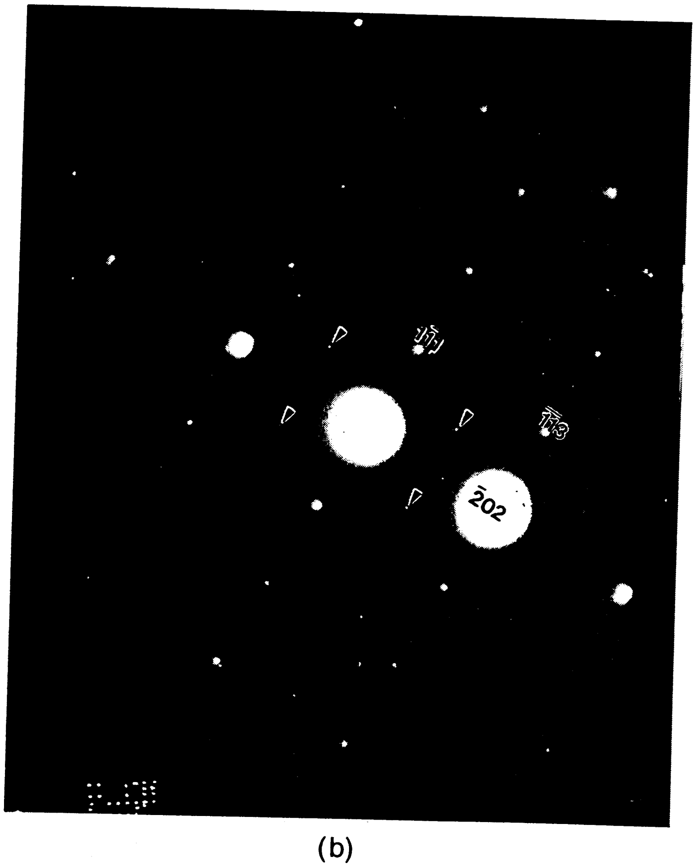
the composites were annealed in a furnace, heating rates and cooling rates were generally limited to tens of degrees per minute. Plan-view TEM specimens were prepared by standard techniques and examined in a Phillips EM420 operating at 120 keV. XRD studies were conducted on a Rigaku x-ray diffractometer equipped with a Cu K_α radiation source and a post beam graphite monochromator to filter K_β radiation intensities.

III. RESULTS

Figure 1(a) is a dark-field micrograph of a 100 nm Ni/(111)Si composite heat-treated for 10 m at 825 °C in a 98% Ar–2% H_2 ambient. The thickness of the nickel silicide film is ~350 nm.[4] The bright regions are epitaxial grains that are of type-B orientation and the dark regions are in type-A orientation. Diffraction patterns from low index poles (i.e., [111]* and [001]*) suggest that these grains are largely composed of $NiSi_2$. However, if the sample is tilted to the [211]* zone axis, there are superlattice intensities at 1/2 {311} positions (referred to Si) in both *type-A and type-B epitaxial $NiSi_2$ grains* [see Fig. 1(b)]. These 1/2 {311} superlattice intensities are observed in the other two ⟨112⟩*-type zone axis accessible to (111) plan-view specimens, i.e., [121]* and [112]*, in both type-A and type-B epitaxial grains. From simple diffraction calculations, these intensities are not permitted in either of the cubic phases of $NiSi_2$ or Si. The presence of these superlattice reflections suggests that an ordered epitaxial phase, based on the Si lattice parameter, may be present within the grains. In electron diffraction studies of plan-view specimens of Ni/(111)Si composites annealed for much longer times (~60 m), these particular reflections are not observed in any ⟨112⟩*-type diffraction patterns. Electron diffraction suggests that only cubic-$NiSi_2$ is formed after long anneals. Thus, it is argued that the ordered structure observed in our films, formed after short anneals, is metastable and is a transitional phase during the formation of the equilibrium $NiSi_2$ phase.

X-ray diffraction studies of Ni/(111)Si samples annealed for 10 m in the temperature range of 650 °C–825 °C also provide evidence of an epitaxial phase present. Figures 2(a) and 2(b) are x-ray diffraction scans of a 100 nm Ni/(111)Si sample annealed for 10 m at 725 °C, again under an argon-hydrogen atmosphere. In Fig. 2(a), the x-ray diffraction scan is centered around Bragg angles of 6.5°–8° ($2\theta = 13°–16°$). In Fig. 2(b), the scan is centered around Bragg angles of 13°–15° ($2\theta = 26°–30°$). The high intensity peaks at $2\theta \sim 28.5°$ in Fig. 2(b) correspond to the peaks of (111)Si. The smaller peak to the right of the Si substrate peaks ($2\theta \sim 28.6°$) corresponds to the (111) diffracted intensity of the equilibrium $NiSi_2$ structure ($d_{111} = 3.13$ Å). This peak is always observed in samples that have been annealed for extended times (>20 m), and TEM studies of such samples show that only $NiSi_2$ exists. The small diffuse peak shown in Fig. 2(a) corresponds to an interplanar spacing of ~6.25 Å. This diffracted intensity does not match any interplanar spacings of Si or $NiSi_2$,

(a)



(b)

FIG. 1. (a) Dark-field TEM micrograph showing type-B epitaxial nickel silicide grains (white regions) and type-A epitaxial grains (background); (b) [121]* diffraction pattern from type-A and type-B $NiSi_2$.

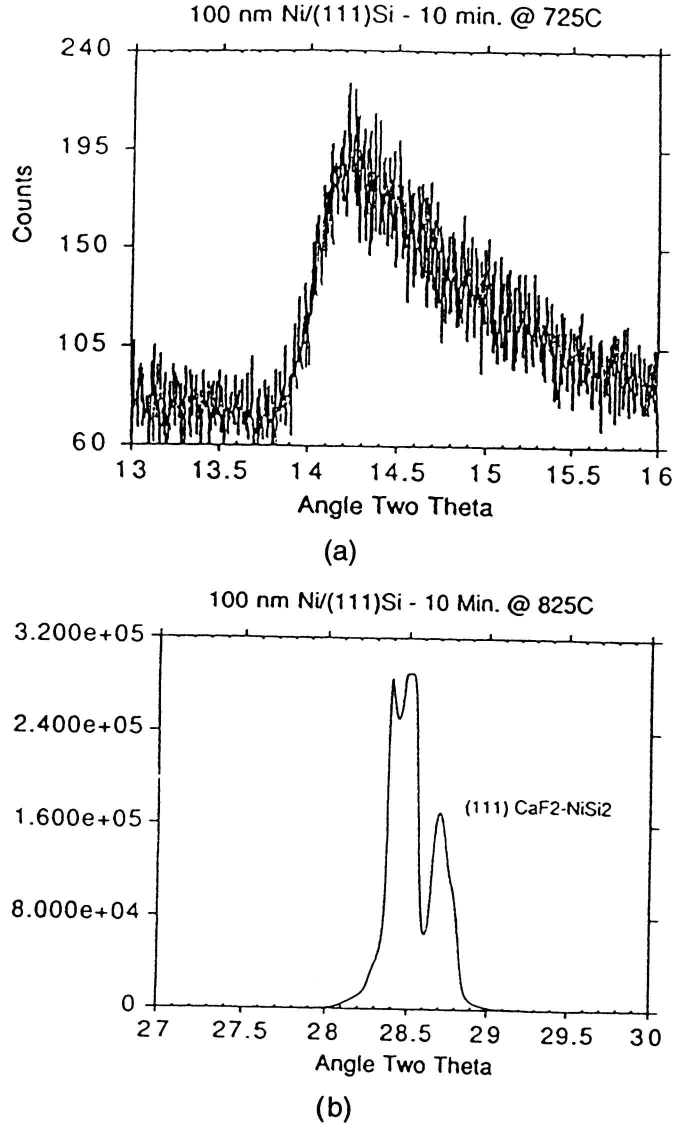


FIG. 2. (a) XRD of 100 nm Ni/(111)Si composite annealed for 10 m at 725 °C taken at $2\theta = 13°-16°$; (b) XRD of 100 nm Ni/(111)Si composite annealed for 10 m at 825 °C.

nor does it match any known interplanar spacings of Ni_2Si or NiSi.[5] The presence of the diffuse peak is believed to originate from an epitaxial nickel silicide phase that possesses a lattice spacing of 10.8 Å. This conclusion is based on the following line of reasoning: In x-ray scans from 2θ of 10°–140°, only three peaks are present. The peaks are observed at (a) 14.2°, (b) 28.6°, and (c) 58.9°. The latter two diffracted intensities originate from the (111) Si (and $NiSi_2$) and (222) Si (and $NiSi_2$) planes, respectively. For small Bragg angles, the quantity $\sin\theta$ approaches that of θ. Thus, the former peak residing at 14.2° is located essentially at half the value of the (111) Si peak. In other words, the diffracted intensity at 14.2° corresponds to a (1/2 1/2 1/2) plane with respect to the silicon lattice. Thus, this particular phase possesses a (111) interplanar spacing twice as large as the (111) spacing for silicon. Hence, the lattice parameter of this epitaxial phase must be twice silicon's lattice parameter (i.e., 10.8 Å).

IV. DISCUSSION

There are two pieces of evidence presented in this work that point to the existence of a metastable epitaxial nickel silicide phase that is produced when annealing thin Ni films with Si: (i) the 1/2 {311} superlattice intensities present in the ⟨112⟩* electron diffraction patterns, and (ii) the diffuse peak in the x-ray scan at 14.2°. Both of these diffracted intensities cannot be accounted for by the presence of a cubic phase such as Si or $NiSi_2$. From a previous study, a structure that may best explain these results is a CuPt-like NiSi structure, but based on the fluorite structure.[3] Figure 3 shows two of the eight fluorite unit blocks, which fully describes

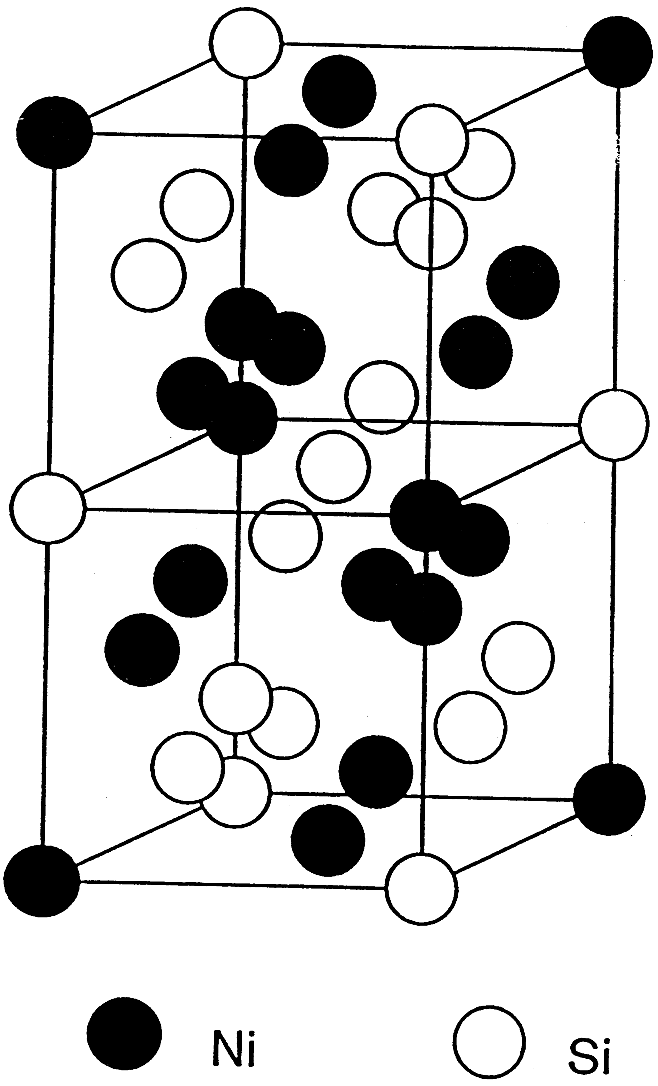


FIG. 3. Schematic drawing of CuPt-like NiSi structure. Only two of the eight fluorite unit blocks that make up the complete CuPt-like structure are shown.

the CuPt-like unit cell structure. The unit blocks, which themselves possess the lattice parameter of Si or $NiSi_2$, are stacked in such a way as to double the lattice parameter along the *x*, *y*, and *z* abcissas. Since the fluorite unit cell contains twelve atoms, the CuPt-like NiSi unit cell contains 96 atoms; thus, the stoichiometry proposed for a perfectly ordered structure is $Ni_{48}Si_{48}$.

Like its fcc counterpart, the (111) planes of a perfectly ordered CuPt-like structure contain only one atomic species, i.e., Ni or Si. The remaining {111} planes contain a mixture of Ni or Si atoms. Variants of this structure have been observed in other TEM foils.[3] However, the epitaxial grains in Fig. 1(a) show evidence of only a single variant with planes of pure Ni and planes of pure Si on planes parallel to the surface. The stacking of the equilibrium fluorite structure, along the [111] direction, can be written as the following: $\underline{A}^{ba}\underline{B}^{cb}\underline{C}^{ac}\underline{A}\ldots$ where the underlined capital letters represent Ni atoms located on the fcc Bravais lattice and the small letters represent Si atoms

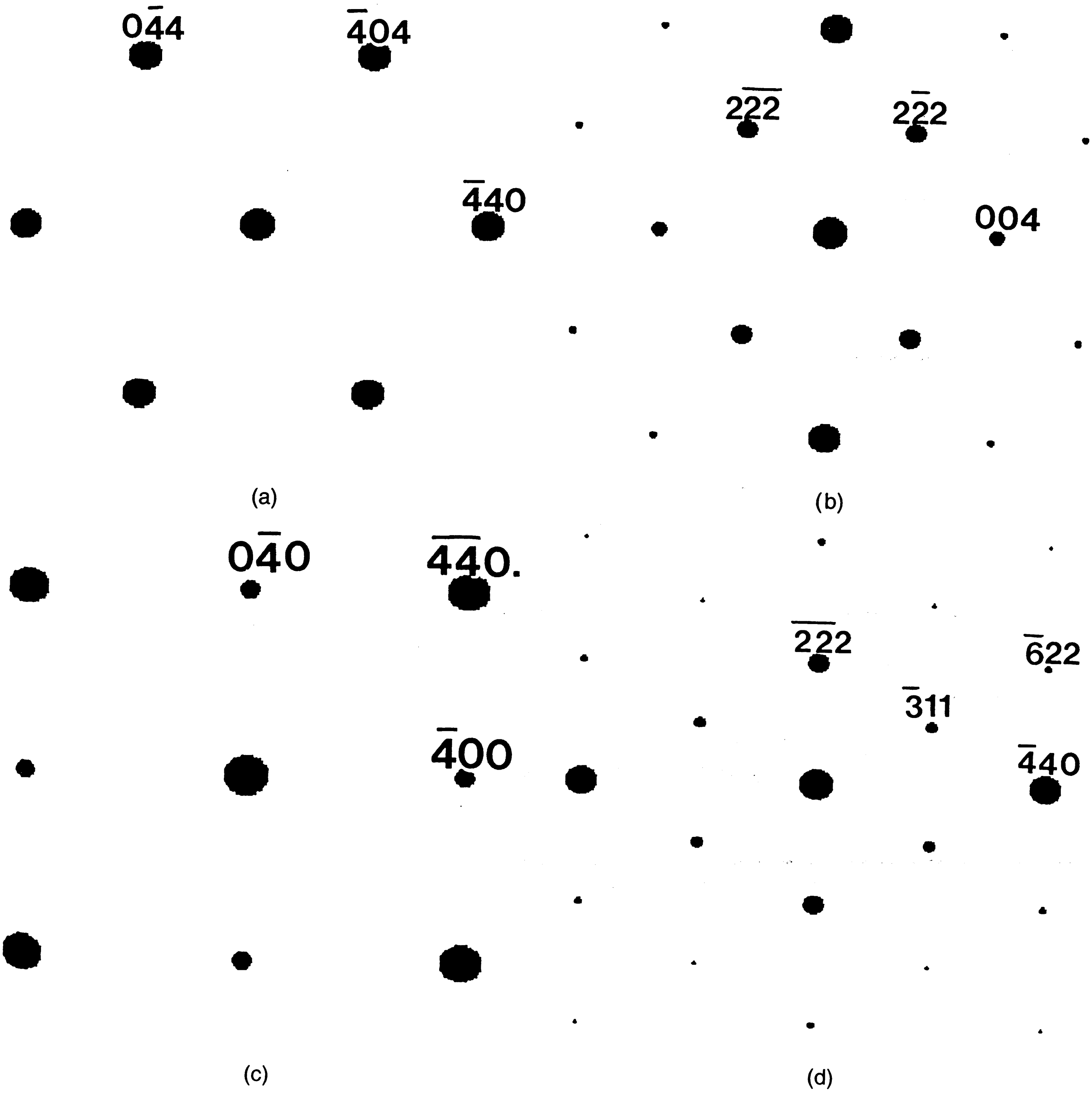


FIG. 4. Computer-simulated diffraction patterns of CuPt-like NiSi: (a) [111]*, (b) [011]*, (c) [001]*, and (d) [112]*.

located at the tetrahedral positions. Nine (111) planes are characteristic of the $NiSi_2$ structure. The CuPt-like NiSi structure has a lattice parameter twice as large as that of Si. Thus, the CuPt-like structure is characterized by 18 (111) layers. The stacking sequence of the (111) planes is proposed to be (with Ni planes underlined): $A^{\underline{b}a}\underline{B}^{c\underline{b}}C^{\underline{a}c}\underline{A}^{b\underline{c}}B^{\underline{c}b}\underline{C}^{a\underline{c}}A\ldots$. Moreover, the (111) planes of the CuPt-like NiSi phase may be considered twin planes for this particular structure.[6] One mechanism of creating type B-NiSi is to "twin" a type-A NiSi structure. This can be accomplished through shears of 1/6 ⟨112⟩ on consecutive (111) planes of NiSi.[6,7]

Computer-simulated diffraction patterns originating from the fluorite-based CuPt-like NiSi phase show excellent agreement with the experimentally observed diffraction patterns. Figures 4(a)–(d) are the computer-simulated [111]*, [011]*, [001]*, and [112]* diffraction patterns expected from CuPt-like NiSi.[8] The diffraction patterns in Figs. 4(a)–4(c) of the rhombohedral structure are observed to be "cubic-like." Indeed, from these patterns, one could conclude that the epitaxial grains contained solely $NiSi_2$. However, the 1/2 {311} reflections in the computer-simulated [112]* diffraction pattern are indicative of the CuPt-like NiSi structure. These particular reflections provide strong evidence that CuPt-like NiSi coexists with $NiSi_2$ in both type-A and type-B epitaxial grains. Table I lists several reflections that are present for the fluorite-based CuPt-like NiSi phase and the calculated structure factor of these reflections.

Several epitaxial nickel silicide films, produced after annealing for short time periods (~10 m) in the temperature range of 650 °C–825 °C, show evidence of the coexistence of the CuPt-like NiSi phase and the equilibrium $NiSi_2$ phase. The diffuseness of the (111) diffracted intensities of the NiSi phase is not fully understood presently. One possible explanation may be due to the fact that the long-range order of this phase is partially destroyed; i.e., the (111) planes of the NiSi structure may be partially intermixed. In addition, since the peak does not appear to be as intense as the (111) $NiSi_2$ diffracted peaks, this observation would suggest that the epitaxial grains consist mostly of $NiSi_2$ and smaller amounts of NiSi. These arguments are consistent with the explanation that the CuPt-like NiSi phase is a metastable phase for the formation of $NiSi_2$. Indeed, x-ray diffraction scans of a 10 nm Ni/(111)Si composite annealed for 10 m at 650 °C show that the NiSi phase exists [Fig. 5(a)] but not $NiSi_2$ [Fig. 5(b)]. Moreover, the metastability of this phase is evident by analyzing films that have been annealed for slightly longer periods. X-ray diffraction scans of Ni/(111)Si samples annealed in the temperature range of 650 °C–825 °C for greater than 10 m show no evidence of the rhombohedral phase, only the presence of cubic-$NiSi_2$. In summary, it is concluded that the CuPt-like NiSi phase is a metastable transitional phase during the formation of "thick" $NiSi_2$. Moreover, because the NiSi phase is found early in the stages of epitaxial nickel silicide phase formation, it is

TABLE I. Structure factor calculations of several NiSi reflections.

NiSi reflection	Reflection referred to Si	Structure factor (F)
(111)	(1/2 1/2 1/2)	$16[1 - 2^{1/2}] \times [f_{Si} - f_{Ni}]$
(311)	(3/2 1/2 1/2)	$16[f_{Si} - f_{Ni}] + 2^{1/2}[4f_{Si}(4 + i) + f_{Ni}(-16 + i)]$
(400)	(200)	$-16[f_{Si} + f_{Ni}]$
(800)	(400)	$48[f_{Si} + f_{Ni}]$

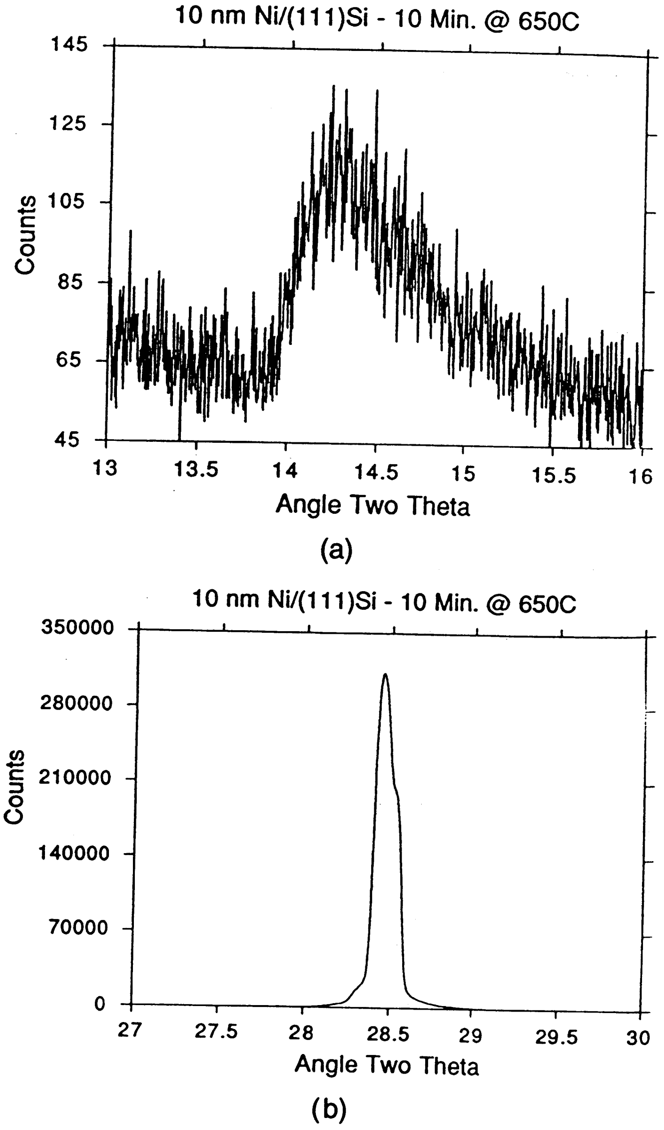


FIG. 5. XRD of 10 nm Ni/(111)Si composite annealed for 10 m at 650 °C: (a) centered around the (111) CuPt-like NiSi peak; (b) centered around the (111) $NiSi_2$ peak.

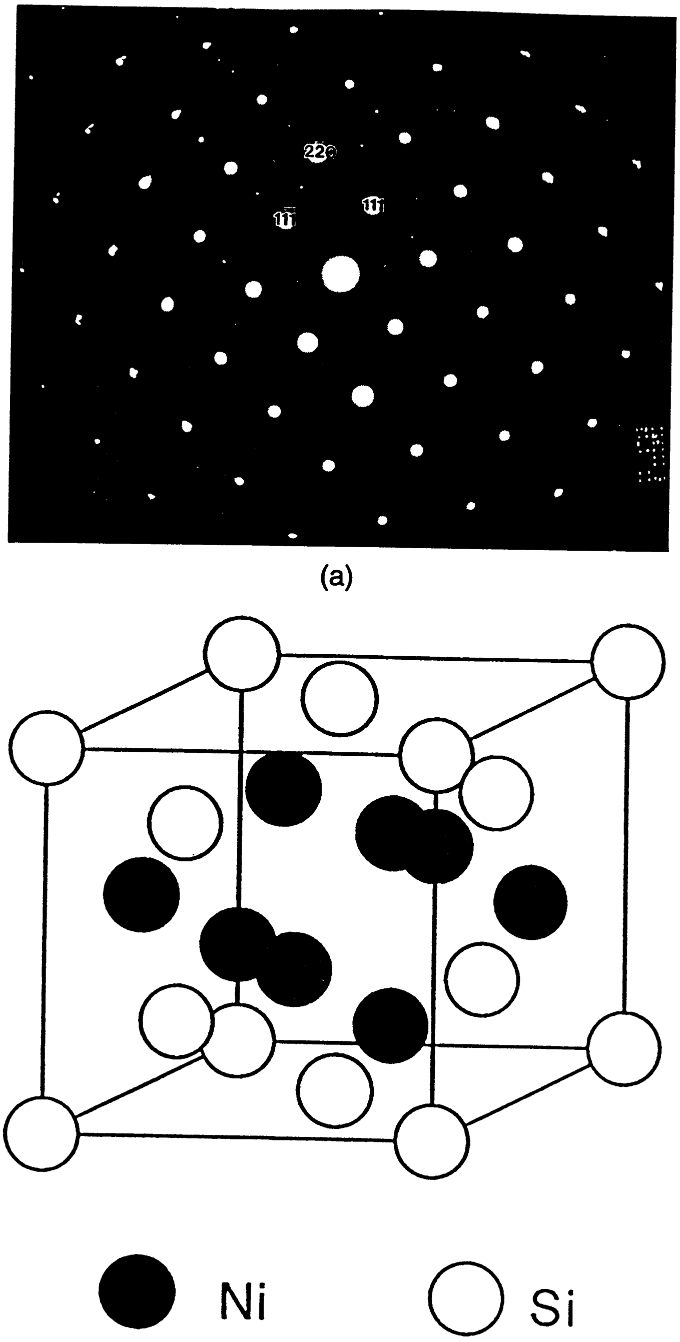
proposed that type-A and type-B orientations are linked to the formation of this rhombohedral structure.

The fluorite-based CuPt-like structure that is proposed in the present work appears to substantiate the results of Baeri *et al.*[9] In their work, they report a thin epitaxial NiSi phase found after pulse laser irradiation. Indeed, strong TEM diffraction evidence was provided to support their hypothesis that the epitaxial material exhibited *threefold symmetry.* As the diffracted intensities for the rhombohedral NiSi phase proposed in the present work closely resemble those of a cubic material, the rhombohedral NiSi phase may be the material created by Baeri *et al.* However, one clear difference between the findings of Baeri *et al.* and that of the present work is the amount of epitaxial NiSi formed. In their films, TEM cross-section micrographs reveal that the entire film is NiSi, whereas the films created in the present work appear to be composed of mostly $NiSi_2$. The difference in the amount of NiSi formed may be linked to the heating and quenching process of Ni/Si composites. Samples examined in the present work were annealed in a three-zone horizontal furnace. The heating rate to the final annealing temperature and cooling rate back down to room temperature is approximately 10 °C–50 °C per minute. Heating and cooling rates after laser irradiation is at least three orders of magnitude higher. The rapid thermal annealing and quenching cycle, inherent in the process used by Baeri *et al.*, may have played a large role in creating the epitaxial film of NiSi.

V. TRANSFORMATION OF FLUORITE-BASED CuAu I-LIKE → CuPt-LIKE STRUCTURES

Figure 6(a) is a [110]* diffraction pattern of an epitaxial grain that was created by annealing a 100 nm Ni/(111)Si couple for 10 m at 825 °C in forming gas. The pattern contains 1/2 {111}, 1/2 {100}, and 1/2 {110} reflections (referred to Si) which are not permitted in Si or $NiSi_2$. The presence of the 1/2 {111} superlattice reflection is indicative of two variants of the fluorite-based CuPt-like NiSi phase. The presence of the 1/2 {100} and 1/2 {110} superlattice reflections reveals the presence of a fluorite-based CuAu I-like structure.[3] Figure 6(b) shows the possible CuAu I-like structure that was previously proposed to coexist with CuPt-like NiSi. This structure is orthorhombic and contains 12 atoms within the unit cell. Previously, it was suggested that the coexistence of the CuAu I-like NiSi and CuPt-like NiSi phases is related to the displacement of Ni or Si along nonequivalent vectors. It was also argued that the CuAu I-like NiSi phase was also a precursor phase to the CuPt-like NiSi phase.[3]

The displacive transformation concept between CuAu I and CuPt—both fcc derivative structures—was originally conceived by Hansson and Barnes[10] and by Pashley *et al.*[7] Figure 7 shows the displacive transformation mechanism proposed by Hansson and Barnes. In Fig. 7(a), CuAu I unit cells are drawn with the "A" and "B" (111) planes outlined by dashed lines. By displacing gray and white atoms to nonequivalent sites [e.g., via a 1/2 [$10\bar{1}$] vector on plane "B"; see Fig. 7(b)], the CuAu I unit cell is now transformed into a CuPt structure with ($\bar{1}\bar{1}1$) layering. Because both CuAu I and CuPt reflections were observed in



(a)

(b)

FIG. 6. (a) [011]* diffraction pattern of epitaxial nickel silicide grain formed by annealing a 100 nm Ni/(111)Si couple for 10 m at 825 °C in forming gas. (b) Fluorite-based CuAu I-like structure.

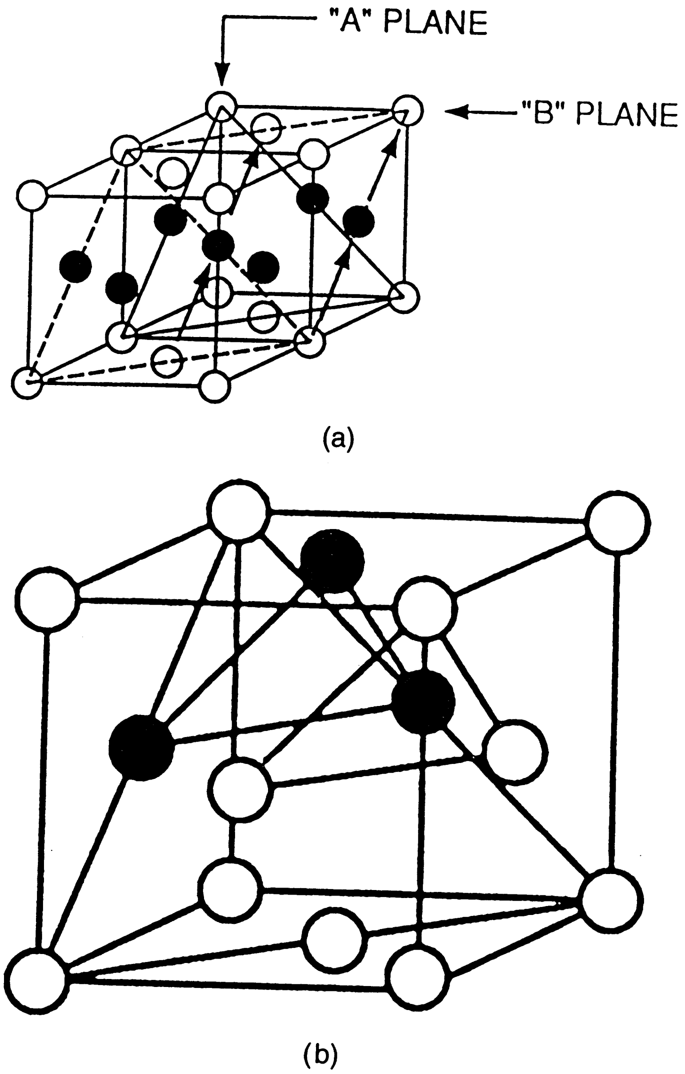


FIG. 7. Displacive transformation concept proposed by Hansson and Barnes for CuAu I → CuPt; (a) CuAu I structure sheared on (111) planes by 1/2 $[10\bar{1}]$; (b) "twinned" CuPt structure.

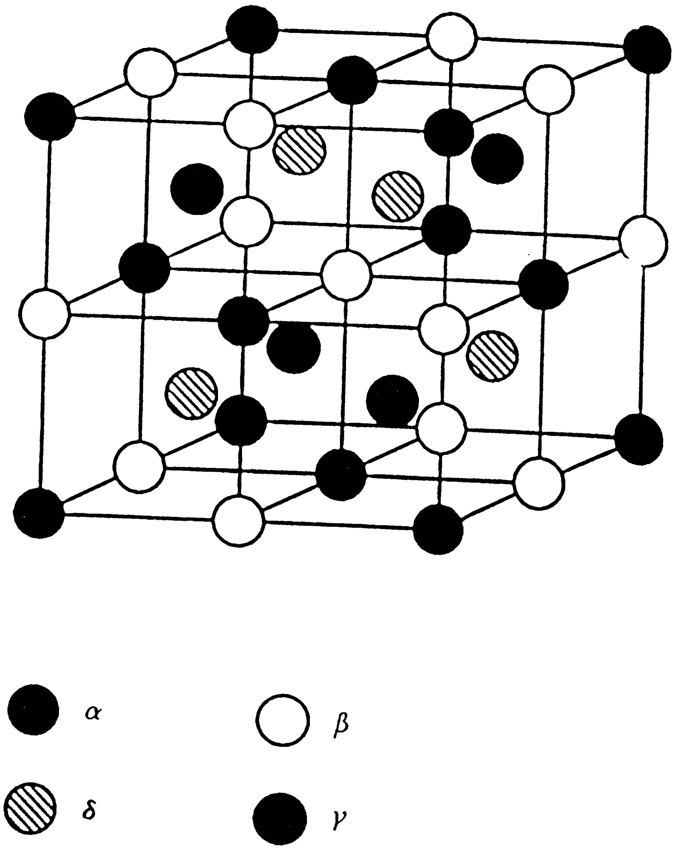


FIG. 8. Sublattice structure of fluorite.

the [011]* diffraction pattern, it is argued that the displacive transformation model is operative in the thin epitaxial films that we have created. However, the fluorite structure is different from the fcc structure since it contains eight tetrahedral sites that are filled with atoms in addition to the four present on the fcc Bravais lattice. Nonetheless, one can extend the original concept of Hansson and Barnes and Pashley *et al.* to rationalize the displacive transformation of the fluorite-based CuAu I-like and CuPt-like structures. In order to understand the interrelationship between the two structures, one must first begin by considering the makeup of the fluorite unit cell.

In a strict sense, the CaF$_2$ structure can be considered to consist of four interpenetrating fcc sublattices (see Fig. 8).[11] Here, the atomic positions of the fcc Bravais lattice, α, are occupied by black atoms. A second fcc sublattice, β, is composed of atomic sites at the body center and halfway along the edges of the α sublattice. These sites are occupied by white atoms. The remaining two sublattices, δ and γ, consist of atoms occupying the tetrahedral sites of Fig. 8. In the schematic drawing, the atomic positions of the δ sublattice are occupied by striped atoms and that of the γ sublattice are occupied by dotted atoms. The NiSi$_2$ structure is constructed by positioning Ni or Si atoms on three of the four sublattices. Ni atoms are positioned on the α sublattice, whereas the Si atoms are positioned on the δ and γ sublattices. The fourth sublattice, β, may be considered to be occupied by vacancies.

Let us consider the manner in which the sublattices are stacked along the [111] and $[\bar{1}\bar{1}1]$ (i.e., twin) directions. The stacking sequence of the sublattices along the [111] direction, for example, follows the sequence: $\alpha\delta\beta\gamma$, $\alpha\delta\beta\gamma$, $\alpha\delta\beta\gamma$, etc. Since in the fluorite structure the β sublattice is filled with vacancies, the stacking sequence can be written as $\alpha\delta\gamma$, $\alpha\delta\gamma$, $\alpha\delta\gamma$, etc. The stacking of the sublattices along the [111] and $[\bar{1}\bar{1}1]$ directions is important when we try to model the structural transformation of the fluorite-based CuAu I-like and CuPt-like NiSi phases.

The fluorite-based CuAu I-like NiSi structure shown in Fig. 6(b) can be considered to be composed of *three interpenetrating fcc-CuAu I units*. The CuAu I unit cell

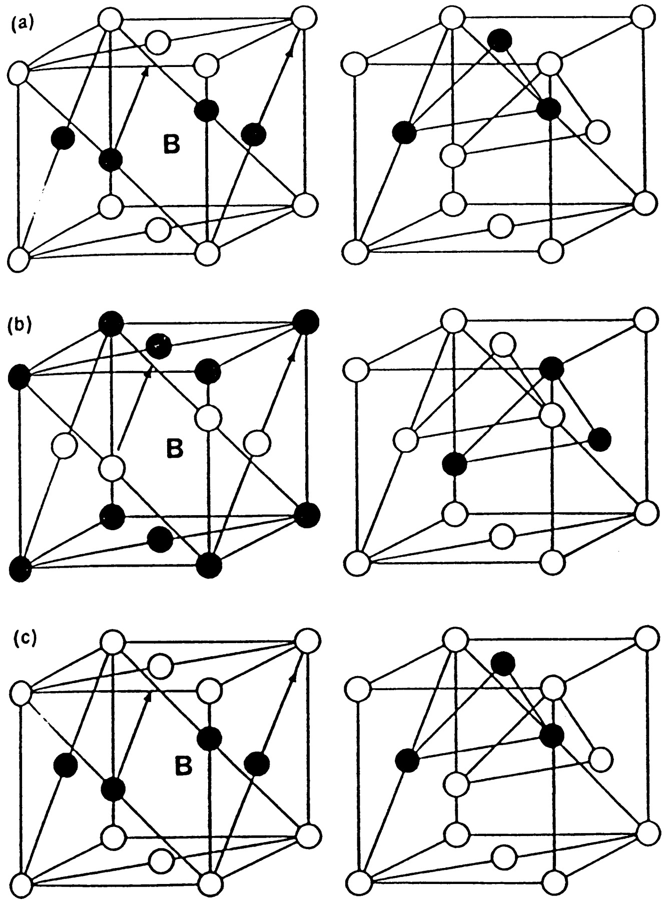


FIG. 9. CuPt structures created by shearing of the CuAu I structures placed on the (a) α sublattice, (b) δ sublattice, and (c) γ sublattice. White circles represent Si atoms, and black atoms represent Ni atoms.

on the fcc Bravais lattice (α sublattice) contains Si atoms at the corners and the {1/2 1/2 0} position and Ni atoms on the {1/2 0 1/2} and {0 1/2 1/2} positions. The CuAu I unit cell on the δ sublattice contains Ni at the corners and {1/2 1/2 0} position and Si atoms on the {1/2 0 1/2} and {0 1/2 1/2} positions. The CuAu I unit cell on the γ sublattice has atoms in the same configuration as the α sublattice.

Let us consider shearing along a nonequivalent vector (e.g., 1/2 $[10\bar{1}]$) on the (111) plane marked **B** in the three CuAu I unit cells [see Figs. 9(a)–(c)]. The shearing of the α–CuAu I sublattice [Fig. 9(a)] creates a CuPt structure on the α sublattice with alternating $(\bar{1}\bar{1}1)$ planes of Si–Ni–Si, etc. In Fig. 9(b), the shearing of the δ–CuAu I sublattice produces a second CuPt structure on the δ sublattice, but here, the layering of $(\bar{1}\bar{1}1)$ planes becomes Ni–Si–Ni, etc. In Fig. 9(c), shearing of the γ sublattice produces the equivalent $(\bar{1}\bar{1}1)$ stacking sequence shown in Fig. 9(a). Recalling that the stacking sequence of the sublattices along the [111] and $[\bar{1}\bar{1}1]$ directions is $\alpha\delta\gamma$, etc., one finds that the stacking sequence produced by the shearing of the CuAu I unit cells becomes Si–Ni–Si–Ni–Si–Ni–Si, etc. We have, in effect, created the $(\bar{1}\bar{1}1)$ variant of the fluorite-based CuPt-like NiSi. This epitaxial NiSi phase is thus composed of *three interpenetrating fcc-based CuPt unit cells.*

VI. CONCLUSIONS

Summarizing our results, we have presented TEM and x-ray diffraction evidence of a single variant of fluorite-based CuPt-like NiSi. This phase exists within epitaxial grains of nickel silicide films after annealing 10–100 nm Ni/(111)Si composites for 10 m in the temperature range of 650 °C–825 °C. The CuPt-like NiSi phase is found only in the early stages of epitaxial film formation. The results in the present work, primarily obtained by electron diffraction and x-ray diffraction, strongly suggest that the type-A and type-B orientations in "thick" (>35 nm) (111) nickel silicide epitaxial films are linked to the formation of "untwinned" and "twinned" CuPt-like NiSi phases. Moreover, the coexistence of fluorite-based CuAu I-like and CuPt-like BiSi has been observed in some TEM samples. A displacive transformation process, based on a model proposed by Hansson and Barnes and Pashley *et al.,* is proposed to occur in these fluorite-derivative structures.

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