indicates the scatter in alignment of the crystallites already discussed.

As always with cross-sectional samples; the diffraction pattern is rather poor. However, it is sufficiently developed now to allow some dark-field work; Fig. 26 shows an example. It is clear that the NiSi-phase is next to the Si-substrate as would be expected.

The implications of these observations shall not be discussed in the context of this paper; for that the reader is referred to / /. Suffice is to say that the bright region separating the silicide layers might be related to oxide remnants, as in the Pd<sub>2</sub>Si and PtSi case discussed before.

# 7.4. Epitaxial NiSi2 on 100 and 111 Silicon Substrates

- Fig. 27 shows cross-sectional micrographs of the NiSi<sub>2</sub> layers formed at 800 °C. The interface is faceted in both cases with facets on 111 and 100 planes, and it is rather "rough" for the NiSi<sub>2</sub> on 100 Si. The silicide surface, too, may be faceted but on a much finer scale (Fig. 27 ). Within a facet, the interface appears to be extremely sharp and absolutely straight.
  - If the specimens are tilted so that the interface is no longer end-on, a dislocation network is visible in the interface (Fig. 2). Whereas this network is observed much more detailed with conventional samples (see before), tilted cross-sectional samples are the better choice if more than one network may be present in various layers of multi-layered structures. This was demonstrated in the case of a Si/CoSi<sub>2</sub>/Si epitaxial structure / /.
  - Fig. 29 shows conventional micrographs of the Si-NiSi<sub>2</sub> interface. In both cases a network of misfit dislocations with spacings in the nm region is present. In the 100 sample the network is quite irregular, consisting mostly of rectangular dislocation

arrangements. Occasionally, more regular square-shaped or hexagonal networks are also observed (Fig. 30 , which shows all three types of networks in comparable proportions, is not typical for the general appearance!). The regular networks can only develop on rather large 100 facets (square network) or 111 facets (hexagonal network). Within most parts of the interface, however, the dimensions of the facets are comparable to those of the network spacing and a large regular network can not be formed.

Using the rules of diffraction contrast, the dislocations can be identified of being edge-type with Burgers vector  $b=\frac{a}{2}$  110; i.e. perfect dislocations as would be expected in this case.

In contrast to the 100 sample; the dislocation network in the Si-NiSi, is very regular. In most regions it consists of a hexagonal network of dislocations with a partial Burgers vector of  $b = \frac{a}{6}$  112; but there are also patches composed of perfect dislocation ( $\underline{b} = \frac{a}{2}$  110 ) forming a hexagonal network with extended dislocation nodes. The basic properties and geometries of such dislocation networks have been described in / will not be detailed here. The geometry of the networks alone would suffice to show that only in the areas containing perfect dislocations the NiSi2 is directly epitaxial to the Si substrate whereas in the regions containing partial dislocations the NiSi, is twinned with respect to the substrate. This twinning of the silicide is not directly evident from the diffraction pattern in Fig. because all major reflections of twinned or untwinned silicide coincide with the Si matrix spots (twinning involves a rotation of 180° around the 111 axis). Fig. shows a weak-beam picture of the network; the dislocation nodes in the area of direct epitaxial growth are clearly visible. These nodes contain a stacking sequence closely related to that of a twinned interface. From the size of the nodes the energy of the "stacking fault" can be calculated / / and is found to have a value of 20 mJ/m<sup>2</sup> / /. This, in a first approximation, can be taken as the energy of the twinned Si-NiSi2 interface and it should be noted that this value is very low.

All the conclusions given above are only true if the misfit dislocations are located exactly at the interface. This is not necessarily so; in principle the networks may be just close to the interface but still completely within the Si or the silicide. There are good arguments that this is not the case (the dislocation nodes, e.g., are too large for dislocations fully contained in Si) but a direct proof would be desirable and this needs high-resolution TEM.

No attempt has been made to detect the misfit-dislocation network that must be present in the 111 Si-NiSi interface because the expected spacing in the order of nm is well below the resolution limit of any CTEM method. Again, only high-resolution TEM (or, perhaps, diffraction-methods, cf. / /) could yield any results in this case.

### 8. <u>High-Resolution TEM and Discussion of the Results</u>

#### 8.1. <u>General</u> Remarks

As already pointed out, HREM requires extremely thin specimens 20 nm) and an extremely precise control of the sample orientation with respect to the electron-beam. These two requirements are almost mutually exclusive for silicide samples. This is so because the stresses invariably present in any Si-silicide interface will cause the sample to bend more or less heavily as the thickness decreases during the specimen preparation procedure. In principle, the goniometer stage of the TEM allows to tilt the sample into any orientation required, but unfortunately only diffraction patterns from moderately thick areas of a specimen allow a control of the established orientation with the needed accuracy. The reason for that is that only if some electrons are inelastically scattered (which precludes HREM), so-called Kikuchi-lines / will be present in the diffraction pattern and these Kikuchilines are needed for precise alignments. The electron-microscopist thus has no choice but to orient the sample by using the diffraction pattern from a thicker part of the specimen as an orientationindicator and then to move to the thin area of interest, hoping

that the proper alignment will not be changed. This hope is often disappointed in bent specimens and attempts to obtain lattice images (not to talk about structural images) can be a frustrating experience.

At the time this paper was written, the structural imaging of silicides and Si-silicide interfaces has just begun; first results may be found in / /. Simple lattice images, however, have been published already / / and they may serve to illustrate the insights that can be gained and the questions that have to be raised by HREM.

## 8.2. Lattice Images of Pd2Si and Si-Pd2Si Interfaces

The first lattice images of silicides have been obtained with conventional specimens of epitaxial Pd<sub>2</sub>Si on 111 Si in 1978 / /; Fig. 34 shows an example. A mosaic structure is clearly visible; the grains are separated by low-angle grain-boundaries (which are necessary to account for small rotations between separate grains), or by stacking-faults and antiphase-boundaries. The latter defects result from the independent nucleation of the Pd<sub>2</sub>Si grains on either an "A", "B" or "C" layer of the Si substrate.

In Fig. the Si substrate was completely removed during specimen preparation. If a thin Si layer is still present, lattice images like the one shown in Fig. result. Predominant contrast features are Moirée fringes resulting from the interference of Pd<sub>2</sub>Si and Si reflections. Fig. shows the early stage of Pd<sub>2</sub>Si growth; only a few epitaxial islands have been formed so far. Particularly suspicious is a "halo" surrounding these islands; the nature of which is not yet quite clear.

Lattice images of cross-sectional specimens are better suited for interface studies than those of conventional specimens. A necessary condition for obtaining lattice-fringes on both sides of the interface is that the Si and the silicide can be oriented into a low-index orientation simultaneously. This restricts lattice imaging

of interfaces to epitaxial systems, or, more generally, to coherent interfaces where at least one set of lattice-planes is continuous across the interface.

This is the case for Pd<sub>2</sub>Si on 111 Si and Fig. shows an example of the Si-Pd<sub>2</sub>Si interface region taken from / /.

More recently, very similar HREM micrographs have also been obtained by Cherns et al. / /; showing that the structures visible in Fig. are "typical" and not only representative. for the peculiar sample investigated. Several features may be noted:

- i) The interface is not faceted and rather wavy on a 2 nm scale.
- ii) The transition from the  $Pd_2Si$  lattice to the Si lattice is atomically sharp in the image; there is no indication of an amorphous layer as suggested in / /.
- iii) A Burgers-like circuit comparing the number of Si 111 fringes and  $Pd_2Si$  2240 fringes does not close; in Fig. there is a surplus of  $Pd_2Si$  2240 fringes.
- iv) The Si lattice close to the interface shows Moirée-like contrast modulations in the form of irregular fringes running about parallel to the interface.

The wavyness of the interface makes it likely that it is not perfectly end-on througout the thickness of the sample which makes the Si-Pd2Si interface less suited for structural imaging. The stacking sequence of Pd2Si is ' ' ' ... and that of Si is Aa Bb Cc... This allows a fairly large number of possible interface configurations (cf. / /) which can be expected to be of different energy. Consider, e.g., the interface: ... AaBb If the silicide grows one more layer the resulting stacking sequence '... and it is unlikely that both interfaces have the same energy (Fig. ). It can be expected that only the low-energy interfaces are realized and this requires either a faceted interface or dislocations which produce a shear in the interface that restores a low-energy configuration. These dislocations are not misfit dislocations because they are required even in misfitfree interfaces. Similar arguments apply to steps in the interface. It the substral surface is not atomically flat, steps must be

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present at least during the early stages of silicide formation and as Fig. 34 shows schematically, steps cannot always be accommodated without introducing some interfacial defect. Obviously, a variety of interfacial defects are needed (including misfit dislocations) to produce a "real" interface and at present it is not all too clear how those defects can be described in a systematic way, how they relate to each other, and what they look like on lattice images.

The lattice image shown in Fig. is not a structural image. For this reason, and because the interface is not perfectly end-on, the sharp transition from the  $Pd_2Si$  lattice to the Si lattice seen on the lattice  $\underline{image}$  does not provide a fully  $\underline{conclusive}$  evidence for an atomically sharp transition of the  $\underline{real}$  lattices. But it is a  $\underline{strong}$  evidence for a sharp interface and any interfacial layer - if present at all - is certainly not thicker than one or two atomic layers.

As shown with the Burgers-like circuit, about every 25th Pd<sub>2</sub>Si 2240 fringe terminates at the interface - the average distance between terminating fringes thus is nm. If the lattice constant of Pd,Si is taken to be nm (that is the measured value from , taking the Si lattice as reference; the tabulated value is nm), a misfit of % is present which could be relieved by a misfit dislocation network having a spacing of it suggests itself to identify the ending 2240 lattice fringes with the misfit dislocations, as done in / /. However, this interpretation, though not completely wrong, is an oversimplification as already noted in / / and also in / /. The correct interpretation of ending lattice fringes in interfaces needs more elaborated treatment; some of the relevant questions will be outlined in chapter 9.

The last point to be discussed is the contrast modulation in the Si lattice image in interface-near regions. It was shown in / / and / / that several possibilities for origin of these contrast features can be ruled out. The most likely explanation is that of a thin layer of a Pd-rich phase overlaying the Si. It is likely that

this overlayer is also related with the "halo" observed around the Pd2Si islands in Fig. . Thin layers covering the Si close to the interface have also been observed in CTEM; Fig. shows an example. Specimens like that shown in Fig. have been investigated with a STEM microprobe / / and it could be shown that the overlayer is Pd-rich (that, incidentially, is the only example of analytical STEM applied to silicides). The origin of the overlayer is not clear at present, but it is likely that it is no intrinsic feature of the Pd2Si-Si interface. It might be caused by corrossive or other processes occurring at the part of the interface exposed to air. Pd atoms, e.g., might migrate (via surface diffusion) to the Si and form Pd2Si there - but that is purely speculative.

### 8.3. Lattice Images of Ni-Silicides

The Ni-silicides are prime candidates for lattice-imaging.

Fig. 35 shows examples of the Si-NiSi2 interface on 100 and 111. Conventional TEM already revealed the faceted nature of these interfaces, but HREM now shows details on an atomic scale. The images are rather poor and represent typical HREM images as they are obtained with heavily bent specimens in one "quick" TEM session. There is no doubt, however, that better images would be obtained if more time could be spent on selecting and imaging suitable specimens. Nevertheless, the following points can be made without over-interpreting the lattice images:

- i) The interface between the Si and NiSi<sub>2</sub> crystal systems is atomically sharp; there is no interfacial layer. The interface is confined to one atomic plane for dimensions of at least 100 nm.
- ii) On 111 substrates the NiSi<sub>2</sub> is in a twin orientation with respect to the Si substrate; the interface constitutes the twin boundary.
- iii) Sometimes the interface contains dislocations which are located exactly at the interface and which produce a step of the interface.

iv) There is a clearly recognizable off-set of the 111 lattice
fringes at the interface (Fig. ).

The last item can serve as a good example of a HREM image feature that must not be interpreted in structural terms. The observed fringe-offset may be completely artificial because the position of fringes with respect to the atom position varies with the sample thickness in a manner which is different for Si and NiSi<sub>2</sub>. This does not exclude the possibility that the fringe off-set is related to structural features of the interface; but without suitable calculations no conclusions should be made.

The confinement of the interface to one atomic plane for rather large areas makes it virtually certain that the interface is exactly end-on in most cases. That is the basic requirement for structural imaging and it is likely that improved HREM images together with calculations based on interface models like the ones shown in Fig. could result in the determination of the precise atomic configuration of the Si-NiSi, interface.

The twinning of the NiSi<sub>2</sub> on 111 substrates is directly visible from Fig. , but easily overlooked with other techniques. Earlier investigations of this interface with Rutherford backscattering in the channeling mode, e.g., did not detect the twinning / /. The twinning has however been confirmed more recently / /, after the TEM results were known, and also found in CoSi<sub>2</sub> grown epitaxially on 111 Si substrates / /.

The lattice images provide good evidence that the misfit dislocations are located exactly at the interface. This, admittedly,
is not all too well visible from Fig. alone; but dislocations
have been observed in other micrographs, too. Fig. , e.g.,
shows the Si-NiSi2 interface on Si, imaged with only that
set of 111 fringes that runs parallel to the interface. The
interface position is only "visible" because the sharp jump in the
mean scattering potential at the interface produces a Fresneltype diffraction fringe at the interface / /. It can be seen
that the interface contains a step of one 111 plane spacing in
height which most likely is due to a misfit dislocation.

The precise location and nature of misfit dislocations is of interest because it is completely unclear how misfit dislocations are generated and move if epitaxial films are formed by solidstate reactions. The situation is different from thin epitaxial films where misfit dislocations, e.g., are generated at the surface and move to the interface by glide and/or climb processes, /. This mechanism cannot be applied to NiSi formation because in this case a thin layer of NiSi, is formed between the substrate and the precursory phase NiSi. Moreover, as the interface advances into the Si-substrate, the dislocations have to follow it and the necessary movement of the dislocations will always have a climb component. Dislocation climb requires emission and/or absorption of as many different kinds of point defects (vacancies and/or interstitials) at the dislocation core as there are different atoms in the crystalline matrix. A climbing dislocation in the NiSi, lattice, e.g., could do so by absorbing Ni and Si vacancies. If only Si vacancies are available, the dislocation might respond by emitting Ni interstitials. That climbing dislocations can indeed disturb the balance of point-defects has been observed in GaAs / / and is likely to happen in silicides as well. Generally speaking, interface dislocations have to interact with the fluxes of point-defects present to drive the silicideforming reaction and in doing so they may change the balance and distribution of point-defects. This, in turn, may alter the reaction kinetics of an epitaxial system compared to a non-epitaxial growth of the same silicide.

The epitaxial system Si-NiSi described in chapter 7.3 has a very large misfit of 15% and therefore would require an extremely dense network of misfit dislocations. If Burgers vectors of  $\underline{b} = \frac{a}{2}$  110 are assumed (corresponding to  $\underline{b} =$  in the hexagonal NiSi) for the misfit dislocations, the spacing of the network would be expected to be nm which makes it unobservable in CTEM. HREM, however, can easily detect the misfit dislocations, Fig. gives an example. The Si 111 fringes and the NiSi 1120 fringes are connected in coherent regions of the interface, but as can be seen very clearly, about every sixth NiSi 1120 fringe terminates at the interface. The spacing of the

terminating fringes thus is just about what is expected for the misfit dislocation network and this observation can be taken as direct evidence for the presence of the postulated misfit-dislocation network although the problems related to interpreting terminating fringes in interfaces mentioned before apply to this case, too.

shows another HREM image of the Si-NiSi interface. This micrograph, as a surprise, clearly shows an "interfacial" layer with a lattice structure very similar to the Si-lattice in other words; a thin layer of epitaxial NiSi2. This intermediate NiSi2 layer was only observed in a few samples taken from the NiSi-covered half-wafer and illustrates the importance of studying several specimens from one system. The Si-NiSi2 interface is already smooth and shows indications of faceting whereas the NiSi2-NiSi interface is quite wavy. After the presence of the thin NiSi<sub>2</sub> layer was established by HREM, it could also be observed in cross-sectional samples using CTEM. The NiSi, layer is too thin to be seen in bright-field, but shows up very clearly if the specimen is imaged in dark-field, using the NiSi, 002 reflection. This is a forbidden reflection for Si (and not existent for NiSi); consequently only NiSi<sub>2</sub> lights up. Fig. gives an example; only a thin layer of NiSi, between the Si and the NiSi is in contrast.

The presence of NiSi<sub>2</sub> in samples annealed at only 400 °C is rather unexpected because it is thought that NiSi<sub>2</sub> does not form below 650 °C / 7. It is possible that the NiSi<sub>2</sub> layer observed would not grow much thicker at the low temperatures and thus would escape detection with practically all investigation techniques. Fig. essentially shows the nucleation of a new phase and further HREM studies of this and similar cases certainly would further our understanding of nucleation and initial growth of silicide phases.

The presence of  $\mathrm{NiSi}_2$  at 400 °C and the formation of epitaxial NiSi at temperatures lower than those for poly-NiSi on 100 substrates may be linked to the extremely high dislocation density

in the epitaxial Si-NiSi interface. Once nucleated, misfit dislocations may speed-up the growth kinetics as described above and also ease the nucleation of the following phase.

### 9. Defects at Interfaces and their Lattice Image

In chapter 8.2. it was already highlighted that "real" coherent interfaces cannot exist without interfacial defects that might be necessary for a variety of reasons. Various kinds of interfacial defects have been described for a number of special cases / /, but no general and systematic classification of interface defects, their specific role in interface geometries and their appearance on lattice images has been given. There is a widespread confusion about these defects which demonstrates itself sufficiently in the rather arbitrary nomenclature found in the literature (cf., e.g./ /). With the advent of direct lattice imaging of interfaces a more systematic treatment of interface defects is urgently needed; this is underscored by emerging discrepancies about the interpretation of lattice-images of Si-silicide interfaces / /.

Within the context of this paper a general theory of interfacial defects cannot be given, but an attempt to classify interfacial defects will be made. The Si-Pd<sub>2</sub>Si interface may serve as a specific example, but the conclusions presented are easily generalized for interfaces of all kinds, including grain-boundaries.

Fig. shows a schematic drawing of possible interface defects in the Si-Pd<sub>2</sub>Si lattice; viewed along the Si 110 direction. In contrast to real Pd<sub>2</sub>Si no misfit is assumed; this serves to demonstrate that even misfit-free real interfaces cannot be defect-free.

Lattice defects need a lattice in which they can exist and in reference to which they are defined. The real crystal lattices are not well-suited as reference lattices because an interface by its very nature constitutes a discontinuity of the lattice. A

lattice particularly well suited for the representation of interface defects is the so-called DSC lattice introduced in the geometric grain-boundary theory of Bollmann / /. For the purpose of this treatment it is sufficient to consider the DSC-lattice as the coarsest lattice constructable that contains the real lattices as sublattices (whereby the real lattices may be strained). The DSC-lattice therefore is continuous across a coherent interface; it is partially drawn in Fig. .

Fig. shows an elementary defect which is called a coherency dislocation in accordance with Olson and Cohen / / because is does not destroy the coherency of the interface (for definition of coherency refer to / / or / /. Coherency dislocations in this case serve to adopt steps in a coherent interface. Real interfaces have steps for several reasons:

- i) The surface of a real substrate is never perfectly flat. If an epitaxial layer is evaporated, the interface must be stepped, too.
- ii) A moving interface, e.g. during silicide growth or during grain-boundary migration, advances by the lateral movement of steps. Steps thus are a necessary ingredient of a moving interface.
- iii) The interaction of lattice dislocations with an interface usually produces a step in the interface.

Coherency dislocations are "real" dislocations because they produce a long-range stress-field identical to that of a common lattice dislocation with the same Burgers vector and, with respect to their TEM contrast, behave like normal dislocations, too. Their movement is restricted to the interface plane (which requires climb if their Burgers rate is not in the interface, cf. / /) but otherwise can be treated like normal dislocation movement processes. If a coherency dislocation is incorporated into an otherwise stress-free interface it will introduce stress. If stresses (e.g. misfit stresses) are already present, coherency dislocations may increase or relieve that stress, depending on the sign of the step that makes their presence necessary. But even

though coherency dislocations <u>can</u> relieve misfit stresses, they should not be confused with misfit dislocations, because their existence is connected with steps in an interface and <u>not</u> with misfit.

A Burgers-circuit around a coherency dislocation done in the DSC-lattice will not close but will give the correct Burgers vector of the coherency dislocation. A <u>Burgers-like</u> circuit, however, comparing corresponding lattice fringes as shown in Fig. , <u>does</u> close. In other words, a coherency dislocation is <u>not</u> associated with terminating Pd<sub>2</sub>Si 2240 or Si 111 lattice-fringes and thus would not be detected in the circuit shown in Fig. .

Clearly, coherency dislocations <u>alone</u> are not sufficient to "construct" a real interface. Misfit, e.g., could only be relieved by coherency dislocations if their associated steps would happen to have the right sign. To give an example: If an epitaxial layer on a substrate with surface-steps is formed by evaporation, both, the sign of the steps and the misfit are independently given and the coherency dislocations needed to accommodate the steps generally will not relieve the misfit stresses, too.

Another independent defect is needed and that is the "pure ledge" shown in Fig. . The name "pure ledge" was chosen in accordance with Hirth and Balluffi / /; the term "coherent step" is also used / /. A pure ledge can be thought as being produced by passing a dislocation through the interface with identical Burgers vectors in both crystals. If a "coincidence-site-lattice" (CSL) / / exists, any CSL-vector will have that property and can be taken as the Burgers vector of the passing dislocation. If no CSL-lattice exists, or if its lattice parameter would be very large; a suitable CSL usually can be found by elastically stressing one of the crystals.

If no misfit is present (corresponding to an exact coincidence position for grain-boundaries), pure ledges are not associated with a long-range strain-field and therefore lack dislocation character. Even a description in terms of dislocation multiples

with vanishing total Burgers vector / / appears to be doubtful because it implies that the pure ledge could dissociate into more elementary defects with dislocation character - which it cannot. Pure ledges destroy the coherency of an interface (therefore the name "coherent step" might be misleading) and, in their "core", contain a piece of an "incoherent" interface; the structure of which in most practical cases is completely unknown. The "core" structure of the pure ledges in Fig. therefore was drawn arbitrarily; the actual structure is not known and anyone's guess. Though lacking dislocation character, a pure ledge is associated with terminating lattice fringes. That is not a paradox because <u>all</u> lattice planes of one crystal terminate at the interface; the apparent continuation is, in a way, a geometric artifact. The  $g \cdot b$  rule in eq. ( consequently can only be applied to vectors of the DSC-lattice. Pure ledges can move by atoms making only a few jumps; i.e. no long-range diffusion is required in mono-atomic interfaces. The interface is advanced by their movement as it is in the case of coherency dislocations, but the mechanisms are basically different (although they may be quite similar in the final analysis of the reaction kinetics).

Coherency dislocations and pure ledges can combine to form defects like the one's shown in Fig. which, in accordance with / /, are called anticoherency dislocations. Exactly like coherency dislocations they can generate (or relieve) stresses, but their step-height is different from that of a coherency dislocation and they are associated with terminating lattice fringes. Drawings shown in the literature usually do not discriminate between coherency and anticoherency dislocations and that is the reason why "one and the same" dislocation might have different step heights, may be "asymmetric" with respect to changing the sign of b; may or may not have ending lattice-fringes associated with it or, vice verse, why sometimes steps going "up" are thought to be associated with an ending lattice plane whereas steps going "down" are not / /.

Within the framework of this paper, the coherency dislocation and the pure ledge are sufficient to construct "real" (i.e. semi-coherent) interfaces. The "common" misfit dislocation, e.g., usually is a perfect lattice dislocation of one crystal but, since any lattice vector can be formed by DSC lattice vectors, can always be composed of coherency dislocations plus pure ledges. Coherency dislocations alone cannot constitute a misfit-dislocation network as will become clear from Fig. A hexagonal network of misfit dislocations is shown which may be taken for the network expected in the Si-Pd, Si interface but, if suitably modified, can also be considered to represent any hexagonal network in any interface with hexagonal symmetry. The hexagons are labelled a, b, c, ... and some of the dislocations are numbered. The roman numerals refer to the interface level with I = paper plane. After choosing the line-directions of the dislocations and giving the sign of  $\underline{\text{one}}$  Burgers-vector  $\underline{\textbf{b}}$ , all the other Burgers vectors can be drawn-in using the node-rule /

Consider now dislocation No. 1 to be the coherency dislocation of Fig. . Then, in going from hexagon a to hexagon b the interface will experience a step and the interface plane is raised from level I to level III. If dislocation No. 2 is a coherency dislocation, too, the interface within hexagon c lies on level V. In going from hexagon c back to hexagon a, the interface must go down from level V to level I. Dislocation No. 3 therefore cannot be a coherency dislocation but must be a combination of the dislocation in Fig. and two pure ledges of Fig. , i.e. an anticoherency dislocation.

Another possible choice for the dislocations could have been:

No. 1 is the coherency dislocation of Fig. ; No. 2 and No. 3

are the anticoherency dislocation of Fig. . It is an interesting question if TEM in the diffraction contrast mode can distinguish between coherency and anticoherency dislocations incorporated in a dislocation network. The contrast is sensitive to the strainfield of the dislocation which is practically identical in both

There are, however, more basic defects as, e.g. the "partial" interface dislocation described by Pond and Smith / /, or dislocation-like defects needed if a CSL can only be found by straining one of the crystals.

cases. However, the "core-structure" is different and it is conceivable that these differences are sufficient to induce detectable contrast differences in special imaging conditions. So far, however, this experiment has not been attempted; it could be tried, e.g., with the misfit dislocation network in the twinned Si-NiSi, interface.

HREM, in principle, can easily distinguish the basic defects.

Burgers-like circuits detecting terminating fringes in connection with a direct observation of the step-height gives, by comparison to Fig. , the precise nature of the defect under investigation (provided it is end-on and structural imaging can be done).

The lattice-image of a hexagonal network can be easily constructed using Fig. and Fig. together. A schematic outline for four different cuts through the two network-cases is given in Fig. . One difficulty is encountered, however: In all cuts (except the cut A-A') the dislocations are no longer end-on. Because eq. ( ) which gives the number of ending fringes for inclined dislocations does not apply to interface defects, it is not clear if inclined anticoherency dislocations are associated with terminating lattice fringes. The problem can be easily solved graphically or by computation of the proper lattice projections.

Without going into a more detailed analysis it can be seen that if ending fringes are observed at all in a cut through a regular hexagonal misfit-dislocation network, they all will be on one side of the interface as is intuitively expected. Their average distance does not give the exact network spacing, but is comparable to it within a factor of perhaps 2 or 3. The tentative interpretation of the terminating fringes with misfit dislocations thus is generally justified, but has to be taken with a grain of salt.

In the specific case of Pd<sub>2</sub>Si on 111 Si, terminating Si 111 fringes can only be observed if the pure ledge shown in Fig. or anticoherency dislocations containing it, are present. Although such defects would not be necessary to accommodate the misfit of the system, they may be present if growth of the silicide is to

proceed by a lateral movement of interfacial defects. Movement of misfit dislocations alone, as suggested in / advance the interface. A regular network can only move as a rigid body which would have no net effect on the interface propagation. Growth can only occur by the constant generation and propagation of anyone of the defects shown in Fig. in addition to the misfit-dislocation network. This process may be visualized, e.g., as adding pure ledges of different sign to neighboring "zig-zag" lines of the network and propagating them in different directions, or by adding any coherency or anticoherency dislocation to the network. The process would correspond to adding an "extrinsic" dislocation to a network of grainboundary dislocations, of, e.g., / /. The movement of this extrinsic dislocation, while advancing the interface, automatically would keep the misfit-dislocation network right at the interface.

At this point the discussion of interfacial defects and their properties shall be ended, although much could still be said. Not treated at all, e.g., were DSC-lattice dislocations with Burgers vector inclined to the boundary plane or misfit in a direction perpendicular to the interface. These and similar issues will certainly receive increasing attention as more and better HREM micrographs of Si-silicide interfaces will be obtained in the near future.