Ballistic electron emission microscopy studies of the $NiSi_2/Si(111)$ interface

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We have performed ballistic electron emission microscopy measurements on the $NiSi_2/Si(111)$ system under UHV conditions. Schottky barrier heights have been measured for types A and B interfaces and are found to be in agreement with other techniques. Through correlations between structural defects in the silicide and local increases in collector currents, we find that elastic scattering in the film can increase ballistic electron transmission rates across the interface.

I. INTRODUCTION

The spectroscopic ability of scanning tunneling microscopy (STM) has enabled detailed investigations of local electronic properties of surfaces for several years now.[1] Recently, a novel application of STM introduced by Kaiser and Bell,[2,3] ballistic electron emission microscopy (BEEM), extends this ability to allow investigation of subsurface electronic properties with high spatial resolution. In BEEM, electrons from an STM are injected into a metal-semiconductor sample and are used to probe the local electronic structure of the buried interface. Electronic properties such as the Schottky barrier (SB) can be quantitatively determined. In addition, the ballistic transport properties of the metal film can be studied. These properties which are sensitive to the microstructure of the film and interface can be expected to vary on a nanometer scale as a result of interfacial chemical reactions, interdiffusion of metal and semiconductor or structural defects.[4]

In this paper, we report the application of BEEM to the investigation of the transport properties of an epitaxial metal disilicide-silicon system, $NiSi_2/Si(111)$. Epitaxial metal disilicide-silicon films such as $NiSi_2$ and $CoSi_2$ can be grown with atomically abrupt and structurally perfect interfaces.[5] $NiSi_2$ is particularly intriguing because two distinct orientations are possible on Si(111): type A, which is in perfect registry with the underlying silicon lattice and type B, which is rotated 180° about the $\langle 111 \rangle$ direction.

Furthermore, electrical measurements by Tung[6] have revealed markedly different SBs between the two types of epitaxy, 0.65 and 0.79 eV for types A and B, respectively. More recently, theoretical calculations by Stiles and Hamann[7] predict dissimilar electron transmission probabilities for the two interfaces. The surprising aspect of this disparity in electronic properties is that the structure of the two interfaces differ only in the position of third and higher nearest neighbors.

Here, we describe BEEM measurements on types A and B and A + B mixed films under ultrahigh vacuum UHV conditions. We observe a local increase in ballistic transmission rates of electrons over the SB near structural defects which we attribute to an increase in elastic scattering in the silicide film. *I-V* spectra indicate values for SB in agreement with those measured with spatially averaging techniques. However, the shape of the spectra do not fit well with the model for BEEM proposed earlier,[3] particularly in the threshold region. A more complex model is needed to describe ballistic transport in this system. A mechanism including energy dependent inelastic scattering has been suggested.[8]

II. EXPERIMENT

The BEEM technique utilizes an STM in constant current mode over a metal-semiconductor sample which is kept at zero bias. The injected electrons travel ballistically into the overlayer, and can pass across the buried interface potential barrier to form a collector current if their energy is high enough. This current is measured either as a function of position as the STM is scanned over the sample surface or measured as a function of sample-tip voltage at a particular point on the sample. We have implemented BEEM in a UHV integrated sample preparation and analysis chambers. The mechanical approach mechanism in our STM is similar to that of Kaiser.[9] We have modified the design for coarse *XY* motion, in UHV sample transfer, *in vacuo* preamps, and tube scanners. The noise limit for collector current measurements is given by the Johnson current noise of the zero biased Schottky junction. To reduce this, we define our device as a window 100 μm square in a field oxide on the silicon. To facilitate a low resistance path to the front side contact, polysilicon is deposited on top of the oxide. We use the Tung template method for growing a thin $NiSi_2$ layer on Si(111).[5]

N-type Si(111) wafers ($n = 8 \times 10^{14}/\mathrm{cm}^3$) are first chemically cleaned,[10] then outgased overnight at 500 °C in UHV. The surface oxide is desorbed at 830 °C in a vacuum of 2×10^{-9} Torr. When samples return to room temperature, an electron-gun is used to evaporate 10–20 Å Ni at a pressure typically of 5×10^{-10} Torr. Heating to 550 °C in the low 10^{-10} Torr range then drives the reaction. Samples are then transferred in UHV to the STM for BEEM measurements. Typically, a tunnel current of 1 nA is used for the BEEM spectra and images. We have characterized the silicides produced with plan-view TEM and found the type of epitaxy produced versus thickness of deposited Ni to agree with Tung.[5] Typical silicide thicknesses produced by this method range from 30 to 60 Å.

III. RESULTS AND DISCUSSION

We first present results of BEEM measurements on $NiSi_2$ films fabricated with an approximately 50% mixture of

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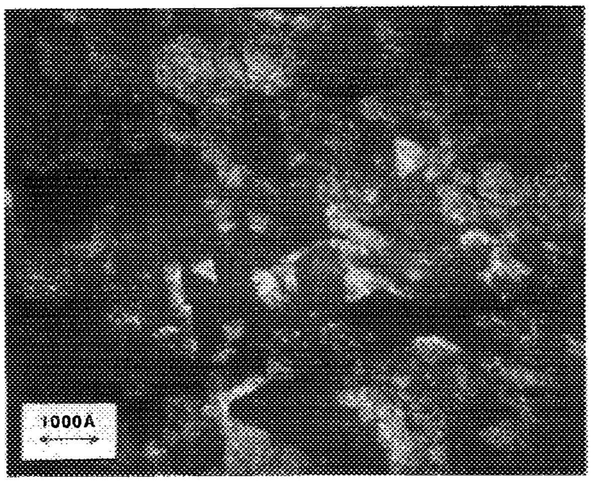

FIG. 1. A 111 dark field transmission electron micrograph of a mixed epitaxy film imaging type-B $NiSi_2$ regions as bright and type A regions as dark.

types A and B grains. TEM studies reveal the grain structure to be highly fractured with individual grain sizes ranging from thousands of Å to tens of Å as shown in Fig. 1. An obvious goal is to image these grains with BEEM so that a direct correlation between the microstructure and electrical properties can be clearly established. If the STM is scanned across a boundary from a type A to a type B grain, one would expect to measure a decrease in the BEEM collector current reflecting the difference in SB for the two types. An STM topograph and simultaneously recorded BEEM image are shown in Figs. 2(a) and 2(b), respectively, for a sample with mixed epitaxy. Atomic ordering of the silicide surface is not visible in the STM topograph due to vibration isolation problems making it difficult to evaluate the quality of the surface. Unless the surface is completely amorphous (i.e., contains no short-range order), TEM studies would be sensitive to disorder. Since this has not been observed, we can infer that the silicide surfaces are, in fact, well ordered. Near a few small structures on the surface as indicated by the arrows, localized increases in collector current can be observed in the BEEM image. This type of correlation is common on all $NiSi_2$ films studied and will be discussed further below. Also discernable in the BEEM image are two distinct areas with different collector current levels separated by a continuous transition region. The transition from one level to the other occurs over several scan lines so we can eliminate a tip switch as the cause. Drift in the current amplifier is also ruled out because such a drift would be measured as an offset current during *I*-*V* measurements. We therefore interpret the transition as indicating a type-A/type-B grain boundary. The current difference is approximately 6 pA between the high and low regions.

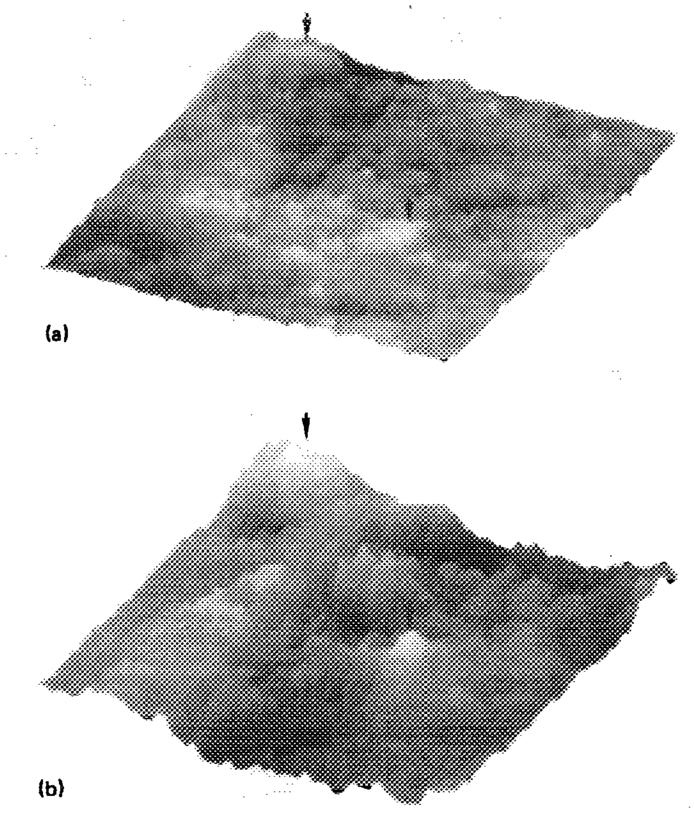

FIG. 2. STM and BEEM images of a $NiSi_2/Si(111)$ sample fabricated with mixed epitaxy. The 200×200 Å^2 STM and BEEM images were acquired simultaneously with a sample-tip voltage of 1.9 V and a 1 nA tunnel current. (a) STM topograph of surface. Grey scale ranges over 10 Å. (b) Corresponding BEEM image which shows a transition from a region of high collector current to a region of low collector current indicating a type-A/type-B grain boundary. Arrows point to small regions of enhanced transmission which are believed to be associated with structural defects in the film. The grey scale covers from 5 to 17 pA.

The BEEM spectra (collector current versus sample-tip bias) for this sample support this interpretation. The two spectra in Fig. 3 were measured at different points and indicate that a major source of contrast in the BEEM images acquired for this sample is due to a shift in SB associated with the presence of both types A and B $NiSi_2$ grains. The difference in current at 1.9 V (the value of sample-tip voltage for the scan in Fig. 2) is 5.5 pA which is close to the difference in the two levels of current measured in the scan in Fig. 2. It is important to note there are other sources of contrast in the BEEM images for these samples. In addition to the observation of enhanced regions associated with topographic features, we also find regions where the collector current is significantly reduced by thickness variations in the $NiSi_2$ film. The combination of these effects tends to convolute the structure observed in the BEEM scan making imaging of individual grains difficult.

The quantitative determination of SBs from the measured BEEM spectra has not been as straightforward as in previous BEEM experiments on Au/Si and Au/GaAs interfaces.[2,3] In those studies, the model first introduced by Bell and Kaiser[3] to calculate the collector current versus voltage was used to fit the BEEM spectra and extract values for the SB. Excellent agreement was found between theory and experimental data for these interface systems. The shape of BEEM spectra measured for the $NiSi_2/Si(111)$ interface, however, is qualitatively different from BEEM spectra mea-

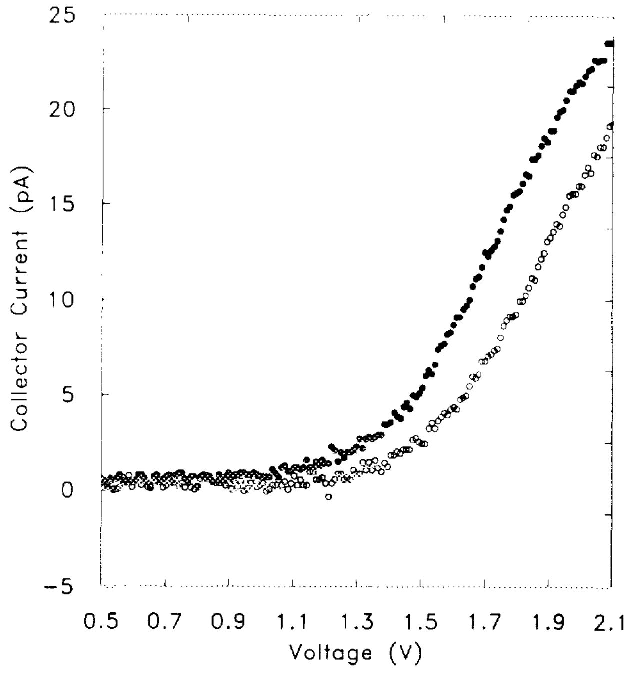

FIG. 3. Two BEEM spectra of collector current vs sample-tip bias measured at different points within a 200 Å square area on the sample imaged in Fig. 2. These spectra indicate that a major source of contrast in the BEEM images acquired for this sample is due to a shift in SB associated with the presence of both types A and B $NiSi_2$ grains.

sured for the other interfaces. Since the model only allows two free parameters, the SB and a scaling factor, fits to the silicide data are poor, particularly in the threshold region. We have found it necessary to modify the model to include an energy dependent transport term to account for this difference. The details of this analysis are described elsewhere,[8] but the essential result is that the BEEM spectra can be used to compute this energy dependent factor which we label as the transmittance. Physical constraints on the transmittance allow us to calculate the SB by an iterative process so that an accurate determination is possible without having an exact functional form for the spectra. It should be emphasized that this is a much more sensitive method of determining the SB than by simple visual inspection of the BEEM spectra. The "square law" dependence of the spectra near threshold is effectively removed in the calculation so that a much sharper turn-on is evident in the transmittance curves.

SB measurements have been made on samples of both types of epitaxy using this method which we estimate to have an uncertainty in absolute value of about 0.02–0.04 eV. We find the types A and B interfaces to have average SBs of 0.71 and 0.84 eV, respectively. These values agree well with those obtained by other techniques.[6] The spatial variation in SB is 0.02 eV for type A samples and 0.03 eV for type B samples which is similar to the variation observed for the Au/Si(100) interface.[2]

As mentioned above, BEEM measurements on all types of $NiSi_2$ films exhibit regions where localized increases in collector current are often observed. These increases usually correlate with topographical features such as surface steps as shown, for example, in Fig. 4. The top image is the standard STM topograph and the bottom image is the BEEM image for an all type B film. Far away from the steps visible in the topograph, the collector current is constant. This suggests that the electronic properties of this interface are spatially homogeneous as in previous BEEM results on the Au/Si(100) interface.[2] Near the steps, however, the collector current is clearly enhanced.[11] BEEM spectra show that this enhancement is associated with an increase in ballistic transmission (the fraction of injected electrons which are collected), and not a decrease in SB. We interpret this change as a local increase in elastic scattering caused by a structural defect in the $NiSi_2$ film. Because the collector current falls to the same value above and below the steps, the steps do not represent a change in the thickness of the silicide film, but instead reflect the topography of the original Si surface. For type B epitaxy, a single (3.14 Å) step in the Si must be accompanied by a partial dislocation in the silicide film as required by symmetry.[12] This type of defect results in a localized strain field in the film which is a source of elastic

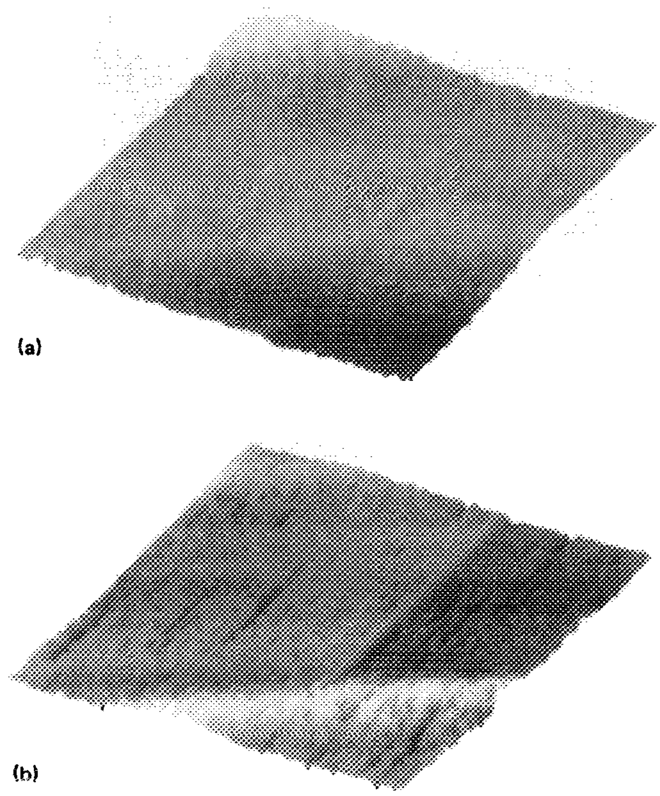

FIG. 4. STM and BEEM images of an all type-B $NiSi_2/Si(111)$ sample recorded with a 1.9 V tip bias and 1 nA tunnel current. The scan area is 175 × 150 Å^2. (a) STM topograph showing surface steps which reflect steps in the underlying Si. The grey range represents 7 Å. (b) corresponding BEEM image showing an enhancement of collector current near the steps. The grey scale covers from 5 to 14 pA.

scattering as evidenced by the fact they can be readily imaged in TEM.[13]

The principle behind this relationship between elastic scattering and ballistic transmission can be understood by first considering the kinematics involved in transport across metal-semiconductor interfaces. For ballistic transport across the interface, transverse momentum and energy are conserved. These conservation laws imply that the transverse wave vector must fall below a certain critical value for transport into the semiconductor conduction band minimum (CBM).[3] For the particular case of transport through a Si(111) interface, there is an additional constraint that the transverse wave vector must be greater than a critical value due to the pronounced offset of the CBM from the center of the Brillouin zone. Because the momentum distribution of the injected electrons is strongly peaked in the forward direction due to nature of the tunneling process from the tip, very few electrons injected into the $NiSi_2$ film have enough transverse momentum to satisfy this constraint. In the absence of elastic scattering in the film, this leads to the conclusion that the transmission through a Si(111) interface should be lower than through a Si(100) interface. However, elastic scattering will act to increase the transverse momentum of the injected electrons. Thus an increase in transmission rates can be expected for transport through a Si(111) interface in regions where elastic scattering is strong. This enhancement effect of elastic scattering thus can explain the increased BEEM currents that we generally observe in the vicinity of structural defects in the $NiSi_2$ film.

IV. SUMMARY

In summary, we have performed BEEM measurements on the $NiSi_2$/Si(111) system under UHV conditions. A boundary between a type-A and a type B grain has been observed on an A + B mixed sample. Schottky barrier heights in agreement with other techniques have been measured and are only slight spatial variations within a single type of silicide is detected. Through correlations between structural defects in the silicide film and local increases in collector currents, we find elastic scattering in the film can increase ballistic electron transmission rates across the interface due to transverse momentum conservation and the conduction band offset of the Si(111) face.

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