Hot Carrier Scattering at Interfacial Dislocations Observed by Ballistic-Electron-Emission Microscopy

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In situ ballistic-electron-emission microscopy (BEEM) has been performed at 77 K on partially strain-relaxed, epitaxial $CoSi_2$/Si(111) films grown by molecular beam epitaxy. Hot electron scattering at individual interfacial dislocations has been observed for the first time by BEEM. Standing wave formation in the metal and changes of the surface electronic structure give rise to significant contrast in BEEM images. Apart from the dislocation- and surface-induced contrast, the interfacial transmission is generally found to be homogeneous.

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The design of modern microelectronic devices such as hot electron transistors and infrared detectors requires the understanding of hot electron transport across a heterointerface. At a perfect interface the transport is based on the conservation of energy and the parallel momentum $k_{\parallel}$. However, the real interface contains point defects, dislocations, and other nanoscale objects. They disrupt the periodicity parallel to the interface leading at the very least to interface scattering, if not to a local change of the band lineup.

The only experimental tool capable of studying hot electron transport with a nm spatial resolution is ballistic-electron-emission microscopy (BEEM) and spectroscopy (BEES) [1]. In its most common application to metal-semiconductor (MS) structures, BEEM uses the tip of a scanning tunneling microscope (STM) to inject hot electrons into a thin metal base. Measuring the fraction of carriers, which is transmitted into the semiconducting substrate, allows one to probe locally the transport in the metal base and the transmission across the interface. Interface scattering, resulting in the violations of $k_{\parallel}$ conservation, has been claimed to be important in several systems such as Cr/GaP(110) [2]. It has also been discussed in conjunction with the striking similarity of the BEEM spectra measured for both Au [3] and Pd [4] on Si(100) and (111). However, direct evidence for electron scattering at individual defects at a MS interface is still lacking. In this low-temperature BEEM investigation on $CoSi_2$/Si(111) we report on a systematic *in situ* study of BEEM current variations in an epitaxial MS system. Hot electron scattering at individual, interface dislocations has been observed for the first time.

Partially strain-relaxed $CoSi_2$ films with thicknesses d between 20 and 72 Å were grown on 3-in. Si(111) wafers by molecular beam epitaxy (MBE). The wafers were n^+ doped (As, $n > 10^{19}$ cm^{-3}) to allow for a simple Ohmic BEEM backcontact by means of a Au-coated spring. In a first step a 1 μm thick, undoped ($n < 10^{15}$ cm^{-3}) Si buffer layer was grown at 700 °C. The silicide was prepared by stoichiometric coevaporation at room temperature (RT) and subsequent annealing at 600 °C [5]. If one uses a template technique, the critical thickness h_c for biaxial strain relaxation is ~40 Å [6]. Even below h_c, relaxed layers can be grown by omitting the template. The diode area of ~2 cm^2 was defined by evaporation through a shadow mask. After growth the samples were transferred to the STM chamber without breaking the UHV. The BEEM measurements were performed at 77 K in a new, low-temperature UHV STM, specifically designed for 3-in. samples [7].

Figure 1(a) displays a typical STM topograph on a 25 Å $CoSi_2$/Si(111) film. The parallel monolayer surface steps are due to the wafer misorientation. The strain is relaxed by a hexagonal array of interfacial dislocations. Their elastic strain field causes a distortion of the surface making the dislocations visible in STM topographs as an array of protruding lines [6]. Most strikingly, in the corresponding BEEM image in Fig. 1(b) the current is sharply increased by ~20% around each dislocation. This is the first direct observation of individual interfacial dislocations by BEEM.

Figure 2 shows cross sections across two dislocation lines. The topography profiles (top) can well be fitted by a Lorentzian, with a full width at half maximum (FWHM) of $2d$ [6], in accordance with elasticity theory. In the BEEM profile (bottom) the current is enhanced by ~10 pA between the two dislocations. The type B symmetry of the interface requires that each dislocation be coupled to an interface step [8]. Therefore, the film has a different thickness between the two dislocations, as will be discussed below.

We have taken BEEM profiles at different voltages and fitted them by a Gaussian, taking account of the contrast between the dislocations by linear background subtraction. The height of the Gaussian rises monotonically from the threshold, reaches a maximum around −1.5 to −2 V and then decreases slowly at higher voltages. By ~−4 V the dislocations are hardly visible in BEEM. The FWHM depends somewhat on the particular tip structure, but it is always much smaller than that of the

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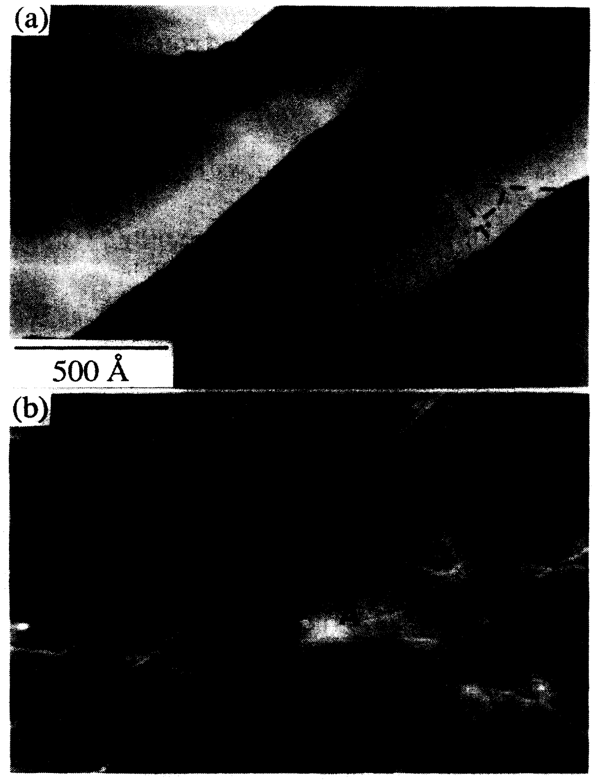

FIG. 1. STM topograph (a) and corresponding BEEM image (b) obtained on a 25 Å $CoSi_2$/Si(111) sample (tip stabilization voltage $V_t = -2$ V, tunneling current $I_t = 5$ nA). The dislocation network is indicated by dashed lines. Region "A" and small stripes parallel to the surface steps exhibit a 2×1 surface reconstruction. In the BEEM image brighter areas indicate regions of higher BEEM current. The arrow indicates an atomic-scale surface point defect (not resolved in the topography image). The typical current variation on the terraces (black to white) is of the order of 50 pA for an average BEEM current of ~200 pA.

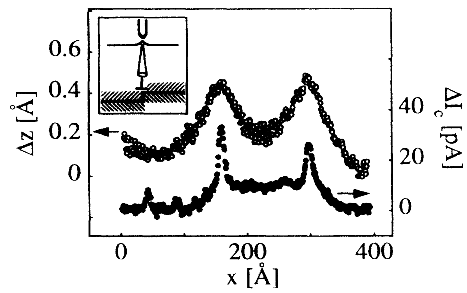

FIG. 2. STM topography (top) and BEEM (bottom) cross sections perpendicular to two parallel dislocation lines, together with a schematic drawing (inset) ($V_t = -1.5$ V, $I_t = 2$ nA, $d = 30$ Å).

corresponding topography. In Fig. 2 it is ≈8 Å. This value is in good agreement with the FWHM, expected if the resolution was limited by the opening angle ϕ_t of the strongly forward focused tunneling momentum distribution [$2d\tan(\phi_t) \approx 10$ Å for a typical value $\phi_t \simeq 10°$]. Therefore, the sharp BEEM profiles imply that the transport in the metal is essentially ballistic, i.e., the tunneling distribution is not significantly broadened by scattering in the metal. The FWHM seems to slightly increase with voltage, probably due to stronger scattering at higher energies, where a larger phase space is available.

The spatially resolved BEES spectra in Fig. 3 were taken right on top of a dislocation ("v") and to its right ("r") and left ("l") in the dislocation-free region. The main spectral features are all similar. The threshold voltage is $\Phi_b = 0.66$ V, close to the Schottky barrier measured by $I(V)$ techniques [9]. We cannot expect to observe any lowering of the potential barrier at the dislocation, since it will be screened ("pinched off") in the undoped Si buffer layer [10]. The spectra exhibit a sharp rolloff from an approximately quadratic [7] to a sublinear behavior around -1.2 V, close to the Si band gap. This has been attributed to electron-hole pair creation at the interface [11]. We observe a distinct high-energy threshold around -1.6 to -1.8 V and a second maximum in the derivative spectra around -2.3 to -2.6 V. The largest difference between the spectra on top and between dislocations is the stronger rise of the BEEM current up to -1.5 to -2 V for the former. On top of the dislocations the current is increased by up to ~60% (at -1.4 V).

The subtle difference between the spectra l and r reflects the steplike contrast observed in the BEEM profiles in Fig. 2. Apart from the difference in film thickness the two surface regions are equivalent, i.e., they exhibit the same sixfold atomic structure of the unreconstructed $CoSi_2$/Si(111) surface. Above ~-2 V,

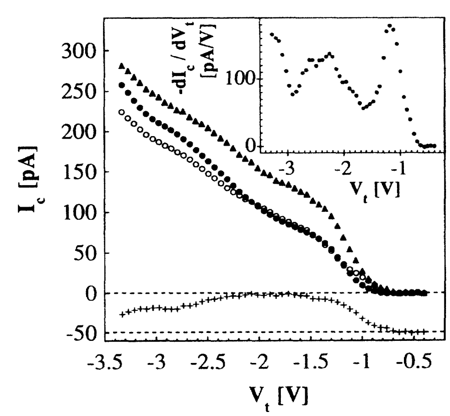

FIG. 3. Spatially resolved constant current BEES spectra on top of a dislocation line "v" (triangles) and at both sides of the dislocation "l" (open circles) and "r" (filled circles), together with the difference spectrum $v - r$ (crosses, displaced by -50 pA). In the inset, the corresponding derivative spectrum for r is shown ($I_t = 3$ nA, $d = 25$ Å).

the contrast increases monotonically but at low voltages it changes sign several times. These small, but reproducible features in the low voltage regime, whose positions depend on the film thickness, are attributed to a quantum interference effect. We have recently observed standing wave formation in the $CoSi_2$ overlayer [12]. Across the dislocation the energy levels of the quantum states are shifted due to the change in film thickness. Contrast in BEEM can be expected, either due to the effect on the metal band structure or simply due to the change of the local density of states (LDOS) at the surface. The latter determines the energy-momentum distribution of the tunneling electrons. In this case, the contrast would be surface induced. It should be noted that the dislocation contrast itself is not a surface effect. Scanning tunneling spectroscopy (STS) did not reveal one-dimensional features in the LDOS, which could correspond to the dislocation lines, visible in BEEM. At higher voltages, the quantum interference disappears [12]. The monotonously increasing contrast at higher voltages might therefore be related to the thickness-dependent attenuation of the BEEM current by scattering.

On an atomic scale, the surface in Fig. 1 is homogeneously unreconstructed. Only in region "A," atomic-resolution STM has resolved a 2×1 surface reconstruction, induced by the thermal stress, developed during cooling from RT to 77 K [7]. In the BEEM image [Fig. 1(b)], the change of the surface electronic structure between the 1×1 and 2×1 gives rise to an increase of the current by ~25% on region A. Atomic-scale surface defects, such as the point defect indicated by the arrow, and scattering at surface steps [13], which are in general not coupled to dislocations, also lead to a larger BEEM current. The resolution is on the atomic scale. It has previously been shown that surface gradients can strongly affect the BEEM current [14]. However, the influence of the surface electronic structure on the tunneling distribution and, hence, the BEEM current has been neglected so far. A detailed discussion on the basis of spatially resolved BEES and STS will be given elsewhere [15].

In Fig. 1(b) the grey scale from black to white corresponds to a small window around the average BEEM current chosen in order to optimally display the dislocation contrast. The typical current variations are smaller than ~25%. In particular, we do not observe patches with almost no current [16]. Apart from the dislocation and surface contrast, the interfacial transmission is generally homogeneous, as expected for an epitaxial interface.

As stated above, the sharp BEEM dislocation profiles imply that the transport in the metal is ballistic. This is corroborated by the observation of the quantum size effect and attenuation length measurements. Therefore, most electrons reach the interface with $k_\parallel \approx 0$. On Si(111) the conduction band minima (CBM) are lying in the $\bar{\Gamma}\bar{M}$ direction ($\parallel \langle 11\bar{2}\rangle$) of the interface Brillouin zone (IBZ), 0.8 $Å^{-1}$ away from the zone center. With respect to the dislocation line ($\parallel \langle 01\bar{1}\rangle$) two of the six CBM lie at an angle of 90°. At the perfect interface, where $k_\parallel$ is conserved, only the small fraction of electrons, injected into states with $k_\parallel$ in the vicinity of the CBM, can be transmitted close to threshold. It is important that the maxima of the topography and BEEM profiles in Fig. 2 exactly coincide. Assuming that the electron states in the metal are localized wave packets traveling in the direction of $\mathbf{k}$, this implies that the electrons contributing to the enhanced BEEM current at the dislocation have $k_\parallel \approx 0$ in the metal. If they travelled in states matching one of the six CBM, i.e., at large angles to the interface normal, one would expect either a much broader profile or even several parallel lines of contrast, displaced with respect to the topography maximum. This leads us to suggest that the main contribution to the dislocation contrast arises from the local violation of $k_\parallel$ conservation. Perpendicular to the dislocation line, the interface periodicity is broken. Interface scattering at the dislocation can provide some of the incident electrons with a momentum component perpendicular to the dislocation, enabling them to enter the CBM. The sharpness of the profiles indicates that the scattering is mainly confined to the dislocation core. The long-range elastic strain field contributes negligibly. In addition, dynamic effects associated with the details of the wave functions at the dislocation might also contribute to the enhanced current.

In order to inquire if core scattering is strong enough to account for the observed contrast, we have performed a simple model calculation. The scattering is treated as a two-step process. First, we calculate the (two-dimensional) differential cross section for elastic scattering from an incoming state $|k\rangle$ with $k_\parallel \approx 0$ into another metal state $|k'\rangle$. Following Harrison [17], the scattering potential is taken to be $V(\mathbf{r}) = \frac{2}{3}E_F =$ const inside the dislocation core. For the subsequent transmission into Si $k_\parallel$ is assumed to be conserved. Within the kinematic BEEM theory [1], the current which adds to that observed in the dislocation-free region is obtained by counting all electrons scattered into the critical angle cones of the Si CBM. Their interface transmission probability (ITP) was set to 1. The calculated excess current exhibits a sharp rise above threshold, due to the enlargement of the critical angle cones. At voltages of -2 to -4 V there is a broad maximum from which on the current decreases slowly, due to the smaller scattering power of the dislocation at higher energies, in qualitative agreement with experiment. For reasonable values of the parameters the maximum calculated current increase is ≈30 pA, per nA tunneling current, close to the experimental value.

The loss of the dislocation contrast at higher voltages can also be understood with the band structure of Si [18]. There are projected zone center Si states, 1.7 eV above $E_F^{CoSi_2}$. Recall that we actually do observe a threshold in the BEES spectrum around that energy (Fig. 3). In the limit, where all states in the IBZ are kinematically allowed with equal ITP, interface scattering should leave the current unchanged. However, even above 1.7 eV, off-centered states can be expected to have a larger ITP due to the larger phase space in Si, whereas the phase space in the zone center only opens up slowly. Together with the finite energy width of the tunneling distribution, this might account for the relatively smooth loss of the dislocation contrast above 1.7 V (see Fig. 3, bottom curve).

Finally, for all film thicknesses, the observed threshold voltage is 0.66 ± 0.05 V, the generally accepted value of the Schottky barrier height [7]. It was determined by fitting the spectra to the kinematic BEEM theory [1,14]. Our value does not agree with the delayed threshold of 0.85 V reported in a previous *ex situ* study [16]. The higher value has been explained by taking into account the calculated $CoSi_2$/Si(111) interface transmission [19]. According to theory, the silicide band structure has no states matching those of the Si CBM. Only 0.2 eV above the CBM do such states become available. To make our results consistent with this calculation, we would be forced to assume another source of scattering at the interface, besides the dislocations, e.g., a high density of interfacial point defects. This could also account for the relatively large current close to threshold, even in the dislocation-free regions. Typical values of I_b/I_t, corrected for attenuation effects, are 0.3%–0.9%, 0.3 V above threshold. This is already of the order of the upper kinematic limit, calculated in kinematic models [1,19], if all electrons injected into the critical angle cones are transmitted (model K_1 in Ref. [19]). A more quantitative statement is difficult, since the current close to threshold may be very sensitive to the unknown tip-to-sample separation [19] (compare spectra *l* and *r* in Fig. 3) and to finite, though small, scattering in the metal and at the surface. The near-threshold spectral shapes on top of and in between dislocations are both close to quadratic [7], although complicated by the quantum size effects. This similarity might be interpreted as another indication for significant interface scattering, since the contribution from scattered electrons can yield a quadratic behavior [4]. However, in the absence of a delayed threshold, the kinematic BEEM theory [1] for Si(111) predicts a slow, but nearly quadratic onset for the unscattered electrons as well, which cannot be easily distinguished from the former. Although the possibility of a spatially uniform contribution from scattered electrons certainly exists, we still feel some reservation against this interpretation. The samples used in our *in situ* experiments were grown by essentially the same MBE technique as in the previous *ex situ* study [16]. Furthermore, the quantum interference effects in our films give evidence for an ordered interface, at which most carriers are specularly reflected. Because our results might also be interpreted as contradicting the existence of a delayed threshold, we prefer to leave a definite answer to a comparison with future experiments on *p*-type Si and $CoSi_2$/Si(100). This problem does not affect the conclusions drawn above. The more observation of the dislocation contrast implies that the momentum distribution cannot be completely randomized, i.e., there must still be a significant fraction of unscattered electrons.

To conclude, hot carrier scattering at individual dislocations, resulting in a sharply localized increase of the current, has been observed for the first time by BEEM. The transport in the silicide is ballistic. In this regime the dislocations can be considered as a "source of parallel momentum," required by the tunneling electrons, to enter the Si. Standing wave formation in the metal layer has been shown to lead to BEEM contrast between regions of different film thickness. Changes of the surface electronic structure, due to different atomic surface structures, can also give rise to significant contrast. We suggest that surface effects should carefully be considered in the interpretation of BEEM images, if one wants to extract the true contribution of interfacial inhomogeneities, especially in the ballistic regime. Apart from the dislocation- and surface-induced contrast, the BEEM current is relatively homogeneous, as expected for an epitaxial interface.

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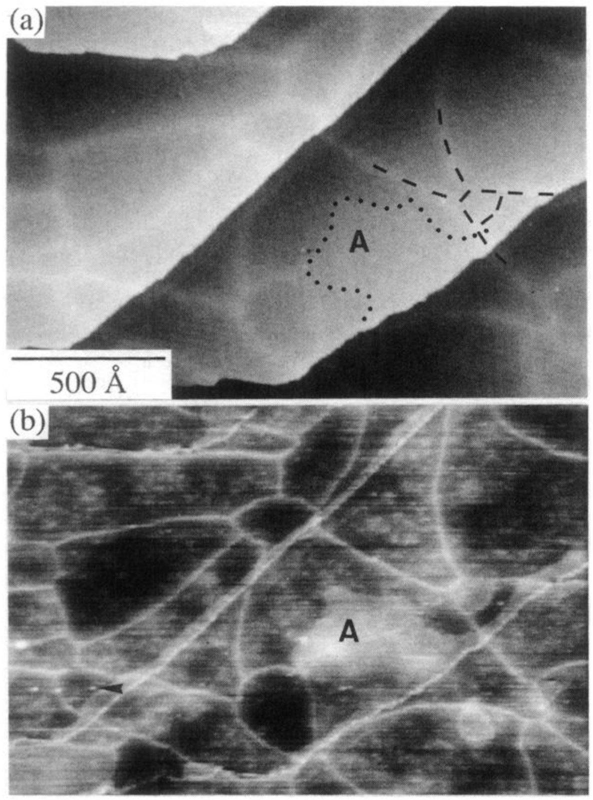

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