Anisotropic scattering of surface state electrons at a point defect on Bi(111)

M. C. Cottin, C. A. Bobisch, J. Schaffert, G. Jnawali, A. Sonntag et al.

Citation: Appl. Phys. Lett. **98**, 022108 (2011); doi: 10.1063/1.3536528
View online: http://dx.doi.org/10.1063/1.3536528
View Table of Contents: http://apl.aip.org/resource/1/APPLAB/v98/i2
Published by the American Institute of Physics.

Anisotropic scattering of surface state electrons at a point defect on Bi(111)

M. C. Cottin,[1] C. A. Bobisch,[1,a)] J. Schaffert,[1] G. Jnawali,[1,b)] A. Sonntag,[1] G. Bihlmayer,[2] and R. Möller[1,a)]
[1]*Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany*
[2]*Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany*

(Received 31 October 2010; accepted 15 December 2010; published online 14 January 2011)

Scanning tunneling microscopy was applied to study the lateral variation of the local density of electronic states on the Bi(111) surface in the vicinity of a point defect. At an energy close to the Fermi level a characteristic pattern with a threefold symmetry is found. The pattern can be attributed to the scattering between two electronic surface states which are split by spin orbit coupling. The observation is well described by the superposition of three monochromatic waves. The phase of the waves relative to the center of the defect leads to a reduction to a threefold symmetry. © *2011 American Institute of Physics*. [doi:10.1063/1.3536528]

The electron transport in metals and semiconductors is an important field of research since it crucially influences the efficiency, the size and the lifetime of electronic components. Recently, bismuth has gained fairly much attention due to its possible application, e.g., in spintronics such as field sensors.[1,2] Bulk bismuth is a semimetal, but it exhibits metallic surface states, e.g., on the (100), (110), and (111) surface.[3–5] It can serve as a prototype system to study transport phenomena within electronic surface states under the influence of strong spin orbit splitting.[6,7] Although for these systems scattering processes connecting the wave vectors $\vec{k}$ and $-\vec{k}$ are forbidden, scattering of the surface state electrons between different wave vectors may result in standing waves of the local density of electronic states, as observed by tunneling microscopy for Bi(110) and Bi(111) as well as for Sb(111).[8–10]

There are theoretical works proposing ultrathin Bi(111) films to be topological insulators.[11–13] These materials have peculiar transport properties.[14] The corresponding band structures have been studied theoretically[15,16] and experimentally by photoelectron spectroscopy[17] for example for $Bi_{1-x}Sb_x$ alloys, Bi_2Te_3 and Bi_2Se_3. Their topological surface states have recently attracted a lot of attention as a base for future electronic applications. They are protected against electronic scattering, even when perturbed by nonmagnetic impurities or other interactions. This has been confirmed experimentally[18,19] as well as theoretically.[20]

In spite of the predicted reduction of scattering processes, it was recently shown that on the Bi(111) surface defects like adatoms or islands have a crucial influence on the conductivity of thin Bi(111) films.[21] The present paper focuses on the analysis of the scattering processes of the surface state electrons at a local defect on a thin Bi(111) film. Particularly, the anisotropy in the variation of the local density of electronic states (LDOS) around the defect will be discussed.

The experiments were conducted in a homebuilt low temperature scanning tunneling microscope (LT-STM) at a base pressure of 5×10^{-10} mbar. During experiments, both, the tip and the sample were cooled to about 80 K by liquid nitrogen using a continuous flow cryostat (Helitran LT-3B). Pt/Ir (90/10) tips were prepared by mechanical cutting and cleaned *in situ* by direct current heating. The Si(111) substrate was cleaned by several cycles of direct current heating to 1500 K, followed by a controlled cooling to room temperature to generate the 7×7-reconstruction. Low energy electron diffraction (LEED) measurements verified the quality of the substrate. A film of Bi(111) with a nominal thickness of about 25 bilayers was epitaxially grown *in situ*.[22] The STM data were acquired using the open source software GxSM[23] and processed using WSxM.[24] All given bias voltages refer to the sample. The dI/dV data were collected using lock-in technique modulating the bias voltage by $\Delta V_{pp}=4$ mV at a frequency of 2 kHz.

Figure 1(a) shows the topography near a step edge and a point defect on the adjacent Bi terrace (marked by a dashed circle). To characterize the size of the defect in more detail, a line profile across the defect and the step edge is displayed in Fig. 1(d). Since the protrusion at the defect is less than 0.5 Å, it can be excluded that it is an island formed by several bismuth atoms because the latter would appear much higher in the STM contour. An individual bismuth atom would diffuse at the given temperature of 80 K. However, the protrusion may be an adsorbate pinned at a dislocation site in the bismuth film. Such dislocations have been observed in images exhibiting atomic resolution.

The scattering of the surface state electrons is revealed by a stationary interference pattern in the LDOS.[25,26] In good approximation the latter is given by the derivative of the tunneling current with respect to the tunneling voltage (dI/dV). Figure 1(b) shows the dI/dV image, which was obtained simultaneously to the topographic image shown in Fig. 1(a). The right side is dominated by the interference pattern of the scattering processes at the step edge. This will be discussed

a)Electronic addresses: christian.bobisch@uni-due.de and rolf.moeller@uni-due.de.
b)Present address: Departments of Physics and Electrical Engineering, Columbia University, New York, NY 10027, USA.

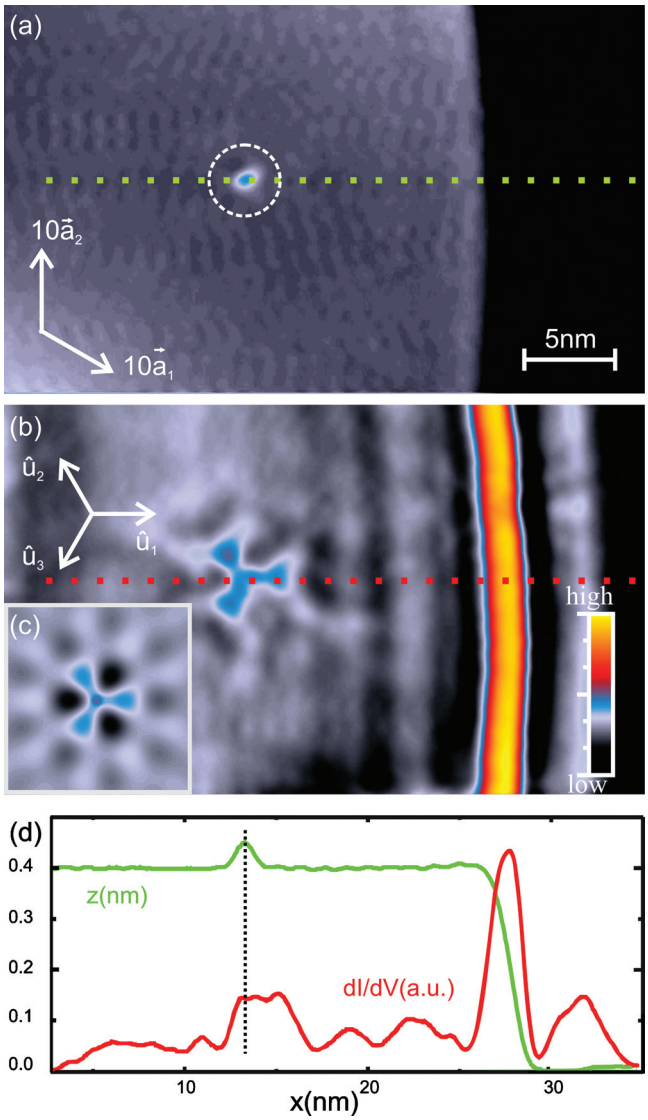

FIG. 1. (Color) STM topography and dI/dV map for a defect and a step edge on a Bi(111) surface. (a) Constant current image of an area of 36 $\times 22$ nm^2; I_t=110 *pA*, V_t=−1 mV, scan speed 40 nm/s, $\vec{a}_{1,2}$ are the base vectors of the surface lattice. The dashed circle marks the point defect. (b) Simultaneously measured dI/dV map, (c) result of a numerical simulation for an area of 12×12 nm^2 around the defect. The scaling corresponds exactly to (b). (d) Line profiles of the topography and the dI/dV signal across the defect and the step edge taken along the dotted lines in (a) and (b).

in greater detail elsewhere. In the middle of the image a starlike pattern with threefold symmetry is found, which is centered at the defect.

To evaluate the contribution of different scattering vectors, a simple numerical simulation based on the superposition of three standing waves was performed. This was realized using the formula[27]

$$\frac{dI}{dV}(\vec{r}) \propto \left[\frac{1}{\sqrt{r^2 + r_{\min}^2}} \sum_{i=1}^{3} \cos(\Delta k(\hat{u}_i \cdot \vec{r}) + \varphi) \right] + C, \qquad (1)$$

where $\vec{r}$ is the position relative to the scattering center, $r_{\min}$ ensures the finite size of the scattering center, Δk is the magnitude of the contributing scattering vectors, $\hat{u}_i$ are the unit vectors as indicated in Fig. 1(b),[28]

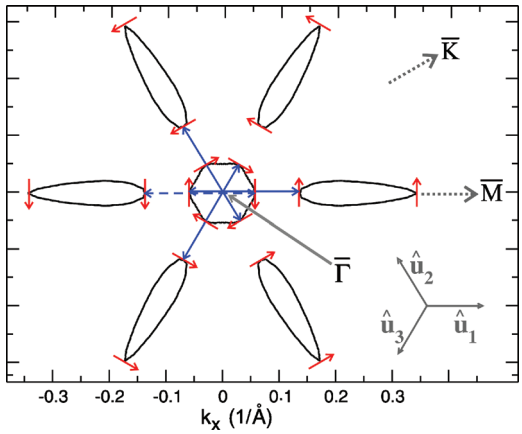

FIG. 2. (Color) Calculated energy contour of the surface states of the Bi(111) surface at E_F. The red arrows display the direction of the spin texture. The blue arrows indicate the transition between the two spin split states (small hexagon in the center and the hole pockets) leading to the observed scattering pattern.

$$\hat{u}_1 = (1,0), \quad \hat{u}_2 = (-1/2, \sqrt{3/4}), \quad \hat{u}_3 = (-1/2, -\sqrt{3/4}),$$

φ is the phase and C is a constant additive factor describing the LDOS of the undisturbed surface. The same pattern is obtained by summing over six plane waves, if the $-\hat{u}_i$-directions are included using $-\varphi$. The simulated image is displayed in Fig. 1(c).

The prefactor warrants that the intensity decays like $1/r$ for large r as expected for a point scatterer in 2D. By replacing r by the geometric mean of r and $r_{\min}$=0.7 nm the expression remains finite for r=0. The exact value of $r_{\min}$ is not crucial. As can be seen by comparing Figs. 1(b) and 1(c), the agreement with the experimental data is surprisingly good given the simplicity of the expression.

A significant parameter of the numerical simulation is the scattering vector, which scales the figures radially. The best agreement to the measurement is found for Δk=0.2 Å^{-1}. There are probably other scattering vectors involved; however, their contribution is of minor importance. The electronic scattering in the surface states of Cu(111) (Ref. 25) or Au(111) (Ref. 26) has been widely studied. For these metals the splitting of the surface state bands results in concentric circular Fermi surfaces around the Γ-point. Between these states the scattering is fully isotropic. In contrast, the Fermi surface of Bi(111) has a sixfold symmetry. Figure 2 shows the Fermi surface calculated using density functional theory in the local density approximation.[7] The calculations are in good agreement with the findings by angle resolved photoemission spectroscopy.[5,29]

From the magnitude and direction of the scattering $\vec{k}$-vectors observed in the interference pattern around the point defect, the processes can be attributed to transitions between the two spin split states as indicated for each direction ($\hat{u}_1$, $\hat{u}_2$, $\hat{u}_3$) by a solid blue arrow. This agrees with the observation for the scattering of surface state electrons on Sb(111).[10] One of the "symmetric processes" is indicated for the $-\hat{u}_1$-direction by the dashed blue arrow.

However, the scattering pattern observed in real space around the point defect only shows a threefold symmetry. This is confirmed by the comparison between the measured data and the numerical simulation shown in Fig. 1(c). The best agreement is found for a phase of φ=1.4 rad≡80°. As

can be seen in the line profile displayed in Fig. 1(d), the resulting oscillation in the LDOS is very asymmetric with respect to the scattering center (at $\varphi=90°$ maximum asymmetry would occur). This shows that the scattering processes of the electron waves propagating with $\vec{k}$ and $-\vec{k}$ are not symmetric with respect to the center of the point defect.

The Bi(111) surface exhibits a threefold symmetry. This is already evident if one considers only the two topmost layers, all following layers do not further affect the symmetry. For a defect which is given by an additional or a missing atom, the nearest neighbor atoms on each symmetry axis of the scattering pattern lie asymmetric around the defect. Thus the periodic surface potential will be perturbed by a potential with a threefold symmetry around the defect. This could explain the phase shift in the oscillation of the LDOS to some extend.

In summary, we have studied the scattering of surface state electrons at a point defect on Bi(111). The findings are of major importance for the understanding of the electric conduction within the electronic surface states of Bi(111). Due to the conservation of the spin and the strong spin orbit splitting the scattering processes are strongly restricted for Bi(111). Hence, a high conductivity would be expected. However, the strong modulation of the LDOS around the defect reveals important scattering processes which correspond to transitions between two different spin orbit split states conserving the spin. This may lead to a significant reduction of the conductivity. The pattern in the LDOS is highly anisotropic exhibiting a threefold symmetry. It reveals that the scattering processes of the electron waves propagating with opposite wave vectors are not symmetric with respect to the center of the point defect.

We thank M. Horn-von Hoegen for fruitful discussions. Financial support is granted by the Deutsche Forschungsgemeinschaft (SFB 616) "Energy Dissipation at Surfaces." M.C.C. and A.S. thank the Studienstiftung des Deutschen Volkes for support.

[1]F. Y. Yang, K. Liu, K. Hong, D. H. Reich, P. C. Searson, and C. L. Chien, Science **284**, 1335 (1999).
[2]K. I. Lee, M. H. Jeun, J. M. Lee, J. Y. Chang, S. H. Han, J. G. Ha, and W. Y. Lee, Mater. Sci. Forum **449–452**, 1061 (2004).
[3]S. Agergaard, Ch. Søndergaard, H. Li, M.B. Nielsen, S.V. Hoffmann, Z. Li, and Ph. Hofmann, New J. Phys. **3**, 15.1 (2005).
[4]M. Hengsberger, P. Segovia, M. Garnier, D. Purdie, and Y. Baer, Eur. Phys. J. B **17**, 603 (2000).
[5]C. R. Ast and H. Höchst, Phys. Rev. Lett. **87**, 177602 (2001).
[6]T. Hirahara, K. Miyamoto, A. Kimura, Y. Niinuma, G. Bihlmayer, E. V. Chulkov, T. Nagao, I. Matsuda, S. Qiao, K. Shimada, H. Namatame, M. Taniguchi, and S. Hasegawa, New J. Phys. **10**, 083038 (2008).
[7]Yu. M. Koroteev, G. Bihlmayer, E. V. Chulkov, and S. Blügel, Phys. Rev. B **77**, 045428 (2008).
[8]J. I. Pascual, G. Bihlmayer, Yu. M. Koroteev, H.-P. Rust, G. Ceballos, M. Hansmann, K. Horn, E. V. Chulkov, S. Blügel, P. M. Echenique, and Ph. Hofmann, Phys. Rev. Lett. **93**, 196802 (2004).
[9]T. K. Kim, J. Wells, C. Kirkegaard, Z. Li, S. V. Hoffmann, J. E. Gayone, I. Fernandez-Torrente, P. Häberle, J. I. Pascual, K. T. Moore, A. J. Schwartz, H. He, J. C. H. Spence, K. H. Downing, S. Lazar, F. D. Tichelaar, S. V. Borisenko, M. Knupfer, and Ph. Hofmann, Phys. Rev. B **72**, 085440 (2005).
[10]J. Seo, P. Roushan, H. Beidenkopf, Y. S. Hor, R. J. Cava, and A. Yazdani, Nature (London) **466**, 343 (2010).
[11]S. Murakami, New J. Phys. **9**, 356 (2007).
[12]S. Murakami, Phys. Rev. Lett. **97**, 236805 (2006).
[13]M. Wada, S. Murakami, F. Freimuth, and G. Bihlmayer, e-print arXiv:1005.3912.
[14]J. E. Moore, Nature (London) **464**, 194 (2010).
[15]H. Zhang, C.-X. Liu, X.-L. Qi, X. Dai, Z. Fang, and S.-C. Zhang, Nat. Phys. **5**, 438 (2009).
[16]L. Fu and C. L. Kane, Phys. Rev. B **76**, 045302 (2007).
[17]Y. L. Chen, J. G. Analytis, J.-H. Chu, Z. K. Liu, S.-K. Mo, X. L. Qi, H. J. Zhang, D. H. Lu, X. Dai, Z. Fang, S. C. Zhang, I. R. Fisher, Z. Hussain, and Z.-X. Shen, Science **325**, 178 (2009).
[18]T. Zhang, P. Cheng, X. Chen, J.-F. Jia, X. Ma, K. He, L. Wang, H. Zhang, X. Dai, Z. Fang, X. Xie, and Q.-K. Xue, Phys. Rev. Lett. **103**, 266803 (2009).
[19]P. Roushan, J. Seo, C. V. Parker, Y. S. Hor, D. Hsieh, D. Qian, A. Richardella, M. Z. Hasan, R. J. Cava, and A. Yazdani, Nature (London) **460**, 1106 (2009).
[20]W.-C. Lee, C. Wu, D. P. Arovas, and S.-C. Zhang, Phys. Rev. B **80**, 245439 (2009).
[21]G. Jnawali, Th. Wagner, H. Hattab, R. Möller, A. Lorke, and M. Horn-von Hoegen, e-J. Surf. Sci. Nanotechnol. **8**, 27 (2010).
[22]T. Nagao, J. T. Sadowski, M. Saito, S. Yaginuma, Y. Fujikawa, T. Kogure, T. Ohno, Y. Hasegawa, S. Hasegawa, and T. Sakurai, Phys. Rev. Lett. **93**, 105501 (2004).
[23]P. Zahl, M. Bierkandt, S. Schröder, and A. Klust, Rev. Sci. Instrum. **74**, 1222 (2003).
[24]I. Horcas, R. Fernández, J. M. Gómez-Rodríguez, J. Colchero, J. Gómez-Herrero, and A. M. Baro, Rev. Sci. Instrum. **78**, 013705 (2007).
[25]M. F. Crommie, C. P. Lutz, and D. M. Eigler, Nature (London) **363**, 524 (1993).
[26]Y. Hasegawa and Ph. Avouris, Phys. Rev. Lett. **71**, 1071 (1993).
[27]If two waves $\psi_1=e^{i\cdot\vec{k}_1\cdot\vec{r}}$ and $\psi_2=e^{i\cdot\vec{k}_2\cdot\vec{r}}$ with different k-vectors interfere, the intensity is given by $|\psi_1+\psi_2|^2\propto\cos^2(\Delta\vec{k}/2\cdot\vec{r})\propto\cos(\Delta\vec{k}\cdot\vec{r})+1$, where $\Delta\vec{k}=\vec{k}_1-\vec{k}_2$.
[28]The direction of $\hat{u}_1$ is given by $\vec{a}_1+1/2\cdot\vec{a}_2$.
[29]C. R. Ast and H. Höchst, Phys. Rev. Lett. **90**, 016403 (2003).