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Local-strain mapping on Ag(111) islands on Nb(110)

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The local in-plane strain of Ag(111) islands on the Nb(110) surface has been derived from the lateral variation of the electronic density of states measured by scanning tunneling spectroscopy. The onset energy E_{ss} of the Shockley-type surface-state band is shifted to higher energies compared to the bulk due to thermal strain arising from the difference in thermal expansion between Nb and Ag and cooling by 565 K. A quantitative dependence of E_{ss} from the strain is obtained by density-functional theory calculations. This allows a mapping of the local strain of individual Ag islands on the nanometer scale. © 2012 American Institute of Physics. [<http://dx.doi.org/10.1063/1.4745011>]

The relation between structural and mechanical properties of thin films and nanoscale objects is a crucial issue for surface applications relying on surface hardness, wear resistance, and friction.¹ In thin films, the total mechanical stress is composed of intrinsic stress and extrinsic stress like thermal stress.² The former arises due to the growth of the film on a substrate and is generated by the epitaxial misfit or by the initial coalescence of individual islands.^{3,4} The latter originates from the difference in thermal expansion coefficients between film and substrate.⁴ The associated thermal strain—averaged over the detected volume—can be studied by x-ray diffraction.⁵ Thermal stress and strain are particularly strong in metals with a low melting point T_m when they are deposited at a substrate temperature $T_S > 0.2 T_m$.² Low- T_m metals have a large thermal expansivity and low energy barriers for diffusion resulting in low intrinsic stresses. The latter might be reduced by recovery due to motion of interstitial atoms, vacancies, and dislocations.

Appropriate objects to study thermal strain ϵ_{th} on the nanometer (nm) scale are metal islands obtained by nucleation and growth on a substrate. Although mechanical stress or strain can be investigated by various surface-science methods including electron microscopy, a mapping of the strain distribution of small objects in real space with nm-resolution is challenging. In this letter, we show that tunneling spectroscopy performed with a scanning tunneling microscope (STM) together with density-functional theory (DFT) calculations allows us to derive a map of the local strain distribution of Ag(111) islands grown on a Nb(110) surface. This is realized by measuring the onset energy E_{ss} of the Shockley-type surface state in the bulk band gap of Ag along the $\bar{\Gamma}-L$ direction. The sensitivity of the surface-state energy on strain, i.e., on the local variation of the electronic structure, has been demonstrated earlier.^{6–8} The obtained strain map is compared with finite-element method (FEM) calculations.

Silver islands were obtained on the surface of a (110)-oriented Nb single crystal (MaTeck GmbH) cleaned by sev-

eral cycles of Ar⁺ sputtering and subsequent heating to 2500 K in ultra-high vacuum. Ag (purity 99.999%) was deposited by electron-beam evaporation at room temperature at a rate of 1 nm/min (≈ 1 monolayer in 18 s) up to a nominal thickness of 5 nm at $T_S = 570$ K ($T_S/T_m = 0.46$). After the sample was cooled down to $T = 5$ K in a single cooling step, scanning tunneling microscopy and spectroscopy (STS) were performed in-situ in a low-temperature STM (LT-STM, Omicron Nanotechnology) with Nanonis electronics. The bias voltage was applied to the sample and $I(V)$ characteristics were taken for voltages $-100 \text{ mV} \leq V \leq +100 \text{ mV}$ at individual points on a 128×128 grid. dI/dV spectra were obtained at each point by averaging over five to ten $I(V)$ curves and subsequent numerical differentiation.

Figure 1(a) shows an STM image of separated Ag islands of 100–300 nm lateral dimension and 10–30 nm height on Nb(110). The island edges are oriented parallel to the Ag $\langle 110 \rangle$ directions. We observe two distinct types of islands: (i) large atomically flat islands (labeled S) with a low density of defects and straight edges enclosing angles

FIG. 1. (a) $2 \mu\text{m} \times 2 \mu\text{m}$ STM image (derivative dz/dx) of Ag islands on Nb(110) at $T = 5$ K (tunneling parameters $V = 100 \text{ mV}$, $I = 100 \text{ pA}$) with indicated crystallographic symmetries of the bcc substrate (white) and fcc island (black). Dashed arrows show the two $\langle 111 \rangle$ directions of the bcc(110) substrate. (b) Topography of a single Ag island on Nb(110) (image size $300 \text{ nm} \times 300 \text{ nm}$). (c) Height profile on top of the island along the arrow shown in (b). Inset shows the profile across the island.

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which are multiples of 60° due to the symmetry of the fcc(111) plane, and (ii) smaller islands (labeled R) with a rough surface and a number of linear defects and edges enclosing angles of 70° or 110° induced by the symmetry of the bcc(110) substrate. Some islands exhibit both types due to coalescence during growth and/or subsequent annealing. The reason for two different types of islands might be the presence of different nucleation sites on the Nb(110) surface and the subsequent growth. The very first few Ag monolayers (MLs) grow in a pseudomorphic fashion on Nb(110) in the Kurdjumov-Sachs orientation with in-plane fcc(110) directions parallel to bcc(111).⁹ Further Ag deposition results in islands (Stranski-Krastanov growth). Due to the twofold symmetry of the bcc(110) surface, two different orientations of fcc(111) islands are observed which are rotated by $\pm 5.3^\circ$ with respect to the bcc [001] direction. Detailed analysis of the sample surface reveals that the Nb(110) surface is covered by 1–2 ML of Ag. This suggests that individual islands are formed during further deposition to reduce the accumulated misfit in nearest-neighbor distances d ($d_{\text{Nb}} = 0.286$ nm, $d_{\text{Ag}} = 0.289$ nm in the Nb(110) and Ag(111) plane, respectively).⁹ Hence, epitaxial strains in the thick islands are considered to be very small. The Stranski-Krastanov growth mode is in agreement with an earlier low-energy electron diffraction (LEED) study of Ag on Nb(110), where the symmetry of the fcc(111) plane was observed for a film thickness exceeding 2 ML,¹⁰ and for Ag(111) on W(110).¹¹

Figure 1(b) shows an STM image of a flat Ag island with two closely spaced parallel linear defects emanating from the island center toward its edge and a third separate parallel linear defect of ≈ 15 nm length. A height profile along the indicated line is shown in Fig. 1(c). The profile shows asymmetric discontinuities. Similar profiles have been attributed to dislocations that produce surface deformations by local strain fields.¹³ In particular, on Ag (111) they have been identified as split-edge dislocations emerging at the surface.⁸ The island has a wedge shape with a thickness that increases from 12 to 17 nm along the horizontal direction (red arrow) due to the parallel alignment of the Ag(111) plane with the Nb(110) plane of the substrate with a miscut of $< 1^\circ$. Apart from the linear defects the surface is atomically flat.

Figure 2 shows (a) $I(V)$ characteristics and (b) dI/dV tunneling spectra obtained with the tip located above the island and away from the island on the 1–2 ML Ag-covered Nb surface. For small tunneling voltages, dI/dV is proportional to the local electronic density of states (LDOSs) with the Fermi level E_F corresponding to zero voltage.¹⁴ On the Ag island, the characteristic step in dI/dV at $V_s = -25$ mV originates from the lower band edge $E_{ss} - E_F = eV_s$ of the quasi-two-dimensional Shockley-type surface state of Ag(111) in the band gap of bulk states along the $\bar{\Gamma} - L$ direction. This contribution is only observed on the atomically flat islands and not on the 1–2 ML Ag-covered Nb surface. The surface state on Ag(111) has been observed frequently in photoemission and STS experiments with $E_{ss} - E_F \approx -65$ meV and an effective electron mass $m^* = 0.4m_e$ (m_e : electron mass).^{15–18} A shift of the surface-state band toward higher energy was found for Ag(111) films on Si,^{6,7} on Ag(111) close to surface steps,⁸ and over buried interfaces.¹⁸ It is attributed to the

FIG. 2. (a) Current-voltage characteristics $I(V)$ acquired with the tunneling tip located on the Nb surface covered by 1–2 ML Ag (blue) and on the 16-nm Ag island (red). (b) dI/dV vs. tunneling voltage obtained by numerical differentiation of $I(V)$.

local change of the electronic band structure of the bulk and surface bands due to lattice strain. The presence of this surface state on the flat Ag islands and the straight edges enclosing multiple angles of 60° confirm that the islands grow along the $[111]$ direction.

In order to directly derive the local strain from the surface-state energy E_{ss} , we have performed DFT calculations of the surface band structure for different in-plane strains. Calculations were performed with the Vienna ab-initio simulation package (VASP) (Refs. 19 and 20) using the projector augmented plane-wave (PAW) method²¹ and the Perdew-Burke-Ernzerhof version of the generalized-gradient approximation for the exchange-correlation potential.²² The strained (111) surface was modeled by a slab of 45 atom layers separated by a vacuum with a thickness of seven layers. The in-plane lattice constant was set to $a = (1 + \epsilon)a_0$, where $a_0 = 0.41645$ nm is the theoretical bulk lattice constant of Ag. For each strain, the slab was allowed to relax in the direction perpendicular to the plane. The large number of layers was necessary to sufficiently reduce the splitting in energy due to the interference between the surface states present on both sides of the slab. We used a plane-wave cutoff energy of 680 eV and a rather dense k -point mesh with 232 points in the irreducible 2D Brillouin zone.

Figure 3 shows the calculated band edges $E - E_F$ for the surface and bulk states at $\bar{\Gamma}$ for different in-plane strains $\epsilon = \Delta a/a$. The splitting of each surface state into a

FIG. 3. Ag(111) surface-state band edge and bulk band edge at the $\bar{\Gamma}$ point vs. in-plane lattice strain obtained from DFT calculations. Open (closed) circles indicate data obtained for the lower (upper) surface of the 45-slab model. Solid lines are linear fits to the data points.

doublet is due to the top and bottom surfaces of the modeled 45-layer slab. For the zero strain, we obtain $E_{ss} - E_F = -35 \pm 7 \text{ meV}$ in reasonable agreement with the experimental value of -65 meV . For the slope of the linear fit to the data, we obtain $\approx 119 \text{ meV}/\%$. The strain dependence of the bulk band edge at the $\bar{\Gamma}$ point shows a somewhat larger slope $\approx 157 \text{ meV}/\%$. A similar dependence of E_{ss} on the lattice strain, i.e., interatomic distance, was suggested earlier from photoemission data on Ag(111) on Si (Ref. 6) where the bands were rigidly shifted upward by 225 meV to reproduce the L'_2 bulk band edge -0.3 eV below E_F .⁶ From photoemission on Ag(111), a temperature dependence $E_{ss} - E_F = -75 \text{ meV} + 0.17 \text{ meV K}^{-1} \times T$ was observed.²³ This corresponds to a shift of the surface state by $90 \text{ meV}/\%$ for $\Delta T = 565 \text{ K}$ estimated by taking into account the thermal expansion coefficient α of Ag ($\alpha_{\text{Ag}} = 18.9 \times 10^{-6} \text{ K}^{-1}$ (Ref. 12)). This value is also in reasonable agreement with our DFT result. In STS on Ag(111)/Si, a decrease of E_{ss} near a dislocation was taken as evidence for the local relaxation of misfits strain in the Ag film around the dislocation.⁷ The strain derived from the shift of E_{ss} is present in the topmost atomic layers due to the small penetration length $\lambda \approx 2.8 \text{ nm}$ of surface states into the bulk.⁶

The fact that V_s is always higher than -65 mV suggests that the Ag islands on the Nb substrate are under tensile in-plane strain, i.e., the Ag (111) lattice plane is expanded with respect to a free Ag film not clamped to a substrate. In the Stranski-Krastanov growth mode, the epitaxial strain in the first 1–2 Ag ML is strongly reduced during subsequent growth by island formation. Therefore, most of the strain observed on the islands is attributed to thermal strain ϵ_{th} generated during cooling the Ag film on the Nb substrate by $\Delta T = 565 \text{ K}$ due to the strongly different thermal expansion coefficients α of Nb ($\alpha_{\text{Nb}} = 7.3 \times 10^{-6} \text{ K}^{-1}$) and Ag ($\alpha_{\text{Ag}} = 18.9 \times 10^{-6} \text{ K}^{-1}$) at room temperature.¹² Because of $\alpha_{\text{Ag}} > \alpha_{\text{Nb}}$ and the clamping of each Ag island to the thick Nb substrate, the island is under tensile thermal strain $\epsilon_{th} > 0$ which can be estimated by,¹

$$\epsilon_{th} = (\alpha_{\text{Ag}} - \alpha_{\text{Nb}})\Delta T = 0.66\%. \quad (1)$$

FIG. 4. dI/dV maps at various tunneling voltages of the Ag (111) island on Nb(110). Image size $300 \text{ nm} \times 300 \text{ nm}$. Color bar: dI/dV in pA/mV .

A detailed calculation of ϵ_{th} must consider the temperature dependence $\alpha(T)$ as done in our FEM calculation, see below.

Fig. 4 shows color-coded maps of the dI/dV value at different tunneling voltages. At -30 mV the shape of the island, cf. Fig. 1(b), is clearly seen. The green-blue background around the island is due to a constant dI/dV value on the 1–2 ML Ag which does not show a surface state. Dark blue color represents regions where the indicated bias voltage V is below the surface-state band edge $E_{ss} - E_F = eV_s$ and a low dI/dV is measured, cf. Fig. 2. If the bias voltage is higher than the surface-state band edge, dI/dV is enhanced due to the additional contribution from the surface states indicated in bright yellow-red color. Hence, the rim where the contrast changes from dark blue to red marks the positions where the tunneling voltage $V = V_s$. In addition, interference patterns are observed near the island edge, for instance the yellow-red regions at the upper left island edge in Fig. 4(c). These are attributed to standing waves arising from the propagation and reflection of surface-state electrons at the island edges or at defects and are frequently observed on metal surfaces at low temperatures.¹⁶ Figure 4 immediately shows that the strain is inhomogeneously distributed at the island surface. In particular, the inner part of the island in the region of the two linear defects is under higher tensile strain than the outer part close to the island rim. This is in contrast to the previous observation of Ag(111) on Si(111) 7×7 indicating a relaxation of strain around the dislocation.⁷ However, it has been pointed out that the shift of E_{ss} can have different signs around edge dislocations.⁸ From the maximal shift of $E_{ss} - E_F$ from -65 meV (Ag single crystal) to $+30 \text{ meV}$ we obtain a strain $\epsilon = 0.8\%$ from our DFT calculation (Fig. 3) in good agreement with the estimated thermal strain $\epsilon_{th} = 0.66\%$, Eq. (1).

With the $E_{ss}(\epsilon)$ dependence at hand, we can map the local mechanical strain of the Ag island by relating the position of the surface band edge E_{ss} to the strain ϵ where lines of constant E_{ss} are considered as isostrain lines. This is shown in Fig. 5(a) where lines of constant in-plane strain ϵ are plotted on top of the STM image. The map visualizes

FIG. 5. (a) Isostrain distribution $\epsilon(x, y)$ derived from the dI/dV maps, cf. Fig. 4. (b) FEM calculation of the stress distribution of the Ag(111) island at $T = 5$ K based on bulk elastic constants. White line indicates the island size at $T_S = 573$ K.

that the strain is enhanced close to the linear defects and relaxes toward the rim. Hence, in the present case the local stress is enhanced close to the dislocation step in contrast to misfit dislocations around which the stress is relaxed.⁷

For comparison of our results with linear elasticity theory, we have conducted FEM simulations and calculated the von-Mises stresses by means of the Comsol Multiphysics package V4.2a with elasticity tensor $\mathbf{c}$ and thermal-expansion coefficients $\alpha(T)$ for Nb(110) on Ag(111).^{24–26} We have used bulk values because there is no evidence that the thermal-expansion coefficient and bulk modulus of a film differ from the bulk values.² Figure 5(b) shows a FEM calculation for an island with a shape adapted to the measured island, cf. Fig. 5(a). The island shrinks when decreasing the temperature from 573 K (white line) to 5 K. The red-colored fringe surrounding the island edge indicates a region of homogeneously distributed stress in the topmost substrate layer. On the island, the stress increases from the island rim toward the center. This is in agreement with our observation that the stress is relaxed at the rim. The variation of strain along the rim is attributed to the anisotropic elastic tensors of the Nb bcc-substrate and the Ag fcc-island.

We conclude that we have demonstrated a mapping of the strain distribution in small Ag islands of submicron size

in real space. This motivates further experiments performed on different film/substrate combinations to investigate the local stress and strain distribution on the nanometer scale.

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