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Supporting Information

The epitaxial growth of ultra-thin palladium films on Re{0001}

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LEED-IV Calculations

Bulk diffraction was calculated using Pendry's layer doubling method for Re bulk inter-layer spacings of 2.23Å. Scattering phase shifts for Re and Pd atoms were calculated as a function of energy using the program package provided by Barbieri and Van Hove. The maximum angular momentum quantum number was set to 9. The imaginary and real parts of the inner potential were set to 4.4eV and -11.4eV (4.1 and -12.8eV), respectively for the clean surface (Pd film). Initially, the radial root mean square displacement for Re and Pd were assumed to be 0.084Å and 0.09Å, respectively. In the final stage of the searches the displacements were optimized together with the inner potential to obtain the best fit between theory and experiment. The

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downhill simplex method was used for the structure optimization\(^2\). RR is the reliability of the R-factor (\(R_P\)),

\[ RR = \sqrt{\frac{8V_i}{\Delta E}} \]

where \(V_i\) is the optical potential and \(\Delta E\) is the total energy range analysed.

**LEED-IV Figures**

The full set of LEED-IV data and best fit curves are given in the following sets of images. For each the title is self explanatory and the black curves the data and the red curves the best fits. Individual \(R_P\) values are indicated for each fit.
Clean Re\{0001\} $3^\circ$ off-normal LEED-IV curves

- (1, -2) $R_p = 0.062$
- (-2, 1) $R_p = 0.050$
- (2, 0) $R_p = 0.141$
- (0, 2) $R_p = 0.096$
- (2, -2) $R_p = 0.191$
- (-2, 2) $R_p = 0.143$
- (-2, 0) $R_p = 0.105$
- (0, -2) $R_p = 0.139$

Energy / eV
Clean Re{0001} -7° off-normal LEED-IV curves

(0,0) Rp = 0.110
(-1,1) Rp = 0.297
(1,1) Rp = 0.099

(0,1) Rp = 0.321
(1,0) Rp = 0.089
(-2,1) Rp = 0.130

(1,-1) Rp = 0.120
(0,-1) Rp = 0.123
(-1,2) Rp = 0.083

Energy / eV

Clean Re{0001} -7° off-normal LEED-IV curves

(2,0) Rp = 0.313
(0,2) Rp = 0.300
(-2,2) Rp = 0.276

Energy / eV
1MLPd/Re{0001} normal incidence LEED-IV curves

(1,0) \( R_p = 0.115 \)

(1,1) \( R_p = 0.204 \)

(2,0) \( R_p = 0.266 \)

1MLPd/Re{0001} off-normal incidence LEED-IV curves

(-1,-1) \( R_p = 0.415 \)

(-1,0) \( R_p = 0.158 \)

(-1,1) \( R_p = 0.057 \)

(0,-1) \( R_p = 0.129 \)

(0,0) \( R_p = 0.240 \)

(0,1) \( R_p = 0.110 \)
1MLPd/Re\{0001\} off-normal incidence LEED-IV curves

\begin{align*}
(1,-2) \quad R_p &= 0.114 \\
(1,0) \quad R_p &= 0.160 \\
(1,1) \quad R_p &= 0.325 \\
(2,1) \quad R_p &= 0.141 \\
(2,-2) \quad R_p &= 0.24 \\
(2,0) \quad R_p &= 0.289
\end{align*}
2MLPd/Re\{0001\} normal incidence LEED-IV curves

(1,0) $R_p = 0.119$

(1,1) $R_p = 0.177$

(2,0) $R_p = 0.205$

2MLPd/Re\{0001\} off-normal incidence LEED-IV curves

(0,0) $R_p = 0.230$

(1,0) $R_p = 0.181$

(0,1) $R_p = 0.179$

(-1,1) $R_p = 0.119$

(-1,0) $R_p = 0.157$

(0, 1) $R_p = 0.177$
2MLPd/Re\{0001\} off-normal incidence LEED-IV curves

- (1,-1) \( R_p = 0.220 \)
- (1,1) \( R_p = 0.224 \)
- (-1,-1) \( R_p = 0.271 \)

- (1,2) \( R_p = 0.155 \)
- (2,0) \( R_p = 0.194 \)
- (2,2) \( R_p = 0.181 \)
3MLPd/Re\{0001\} normal incidence LEED-IV curves

\[(1, 0) \quad R_p = 0.16\]

\[(1, 1) \quad R_p = 0.150\]

\[(2, 0) \quad R_p = 0.239\]

3MLPd/Re\{0001\} off-normal incidence LEED-IV curves

\[(0, 0) \quad R_p = 0.194\]

\[(1, 0) \quad R_p = 0.197\]

\[(0, 1) \quad R_p = 0.179\]

\[(-1, 1) \quad R_p = 0.039\]

\[(-1, 0) \quad R_p = 0.222\]

\[(0, 1) \quad R_p = 0.207\]
3MLPd/Re\{0001\} off-normal incidence LEED-IV curves

(1,1) \( R_p = 0.200 \)

(-1,-1) \( R_p = 0.222 \)

(1,-2) \( R_p = 0.222 \)

(2, 1) \( R_p = 0.171 \)

(2, 0) \( R_p = 0.209 \)

(2, -2) \( R_p = 0.284 \)
4MLPd/Re\{0001\} normal incidence LEED-IV curves

- \((1,0)\) \(R_p = 0.093\)
- \((1,1)\) \(R_p = 0.153\)
- \((2,0)\) \(R_p = 0.046\)

4MLPd/Re\{0001\} off-normal incidence LEED-IV curves

- \((0,0)\) \(R_p = 0.117\)
- \((1,0)\) \(R_p = 0.197\)
- \((0,1)\) \(R_p = 0.100\)
- \((-1,1)\) \(R_p = 0.088\)
- \((-1,0)\) \(R_p = 0.135\)
- \((0,1)\) \(R_p = 0.222\)

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Supplementary References

