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Epitaxial growth of ultrathin palladium films on Re{0001}

Article

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Supporting Information

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

Haitham A. Etman, Zhasmina V. Zheleva, Georg Held and Roger A. Bennett[a]

School of Chemistry, University of Reading, Reading, RG6 6AD, UK

LEED-IV Calculations

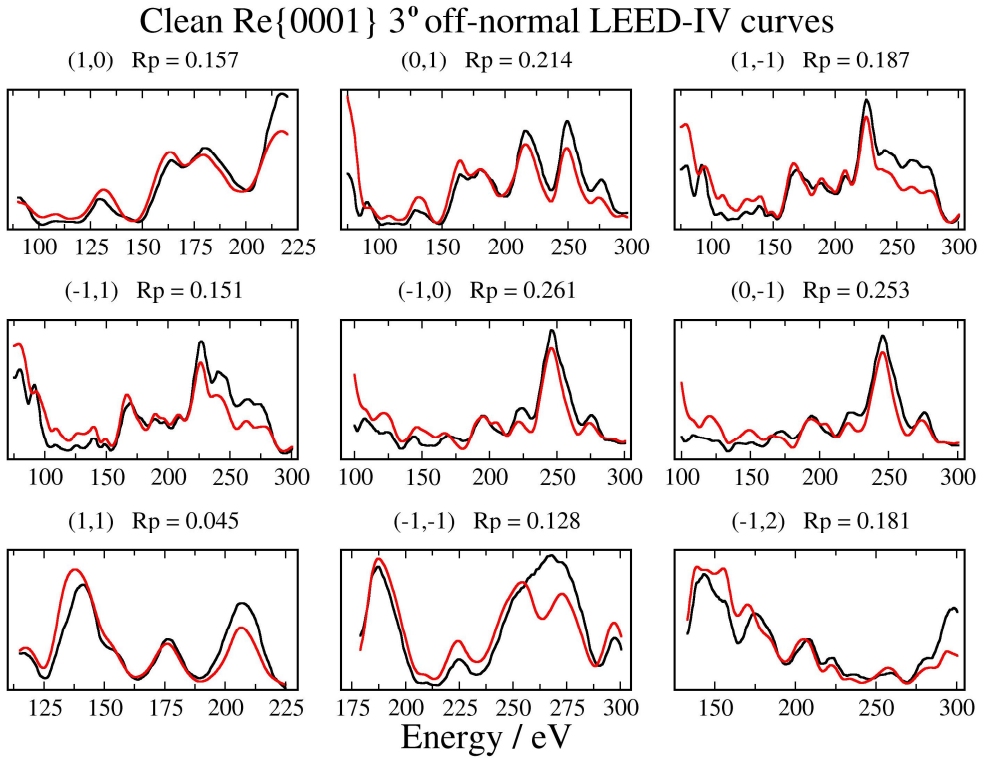
Bulk diffraction was calculated using Pendry's layer doubling method for Re bulk inter-layer spacings of 2.23Å. Scattering phase shifts for Re and Pd atoms were calculated as a function of energy using the program package provided by Barbieri and Van Hove[1]. The maximum angular momentum quantum number 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

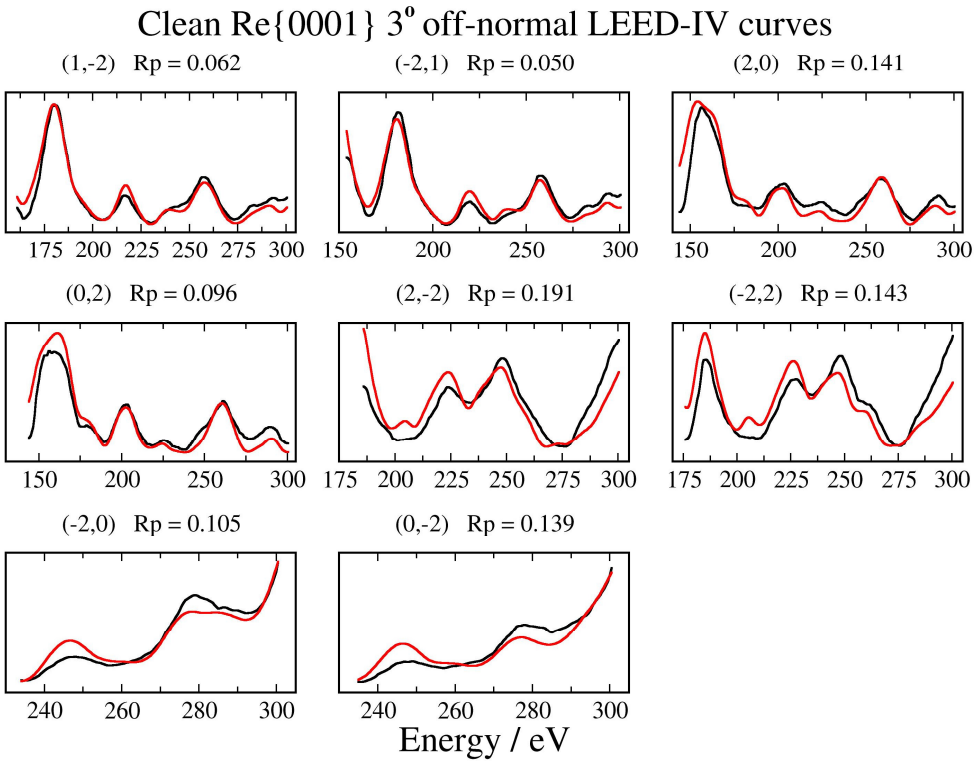
[a] E-mail: r.a.bennett@reading.ac.uk, Telephone: +44 (0)118 378 8559

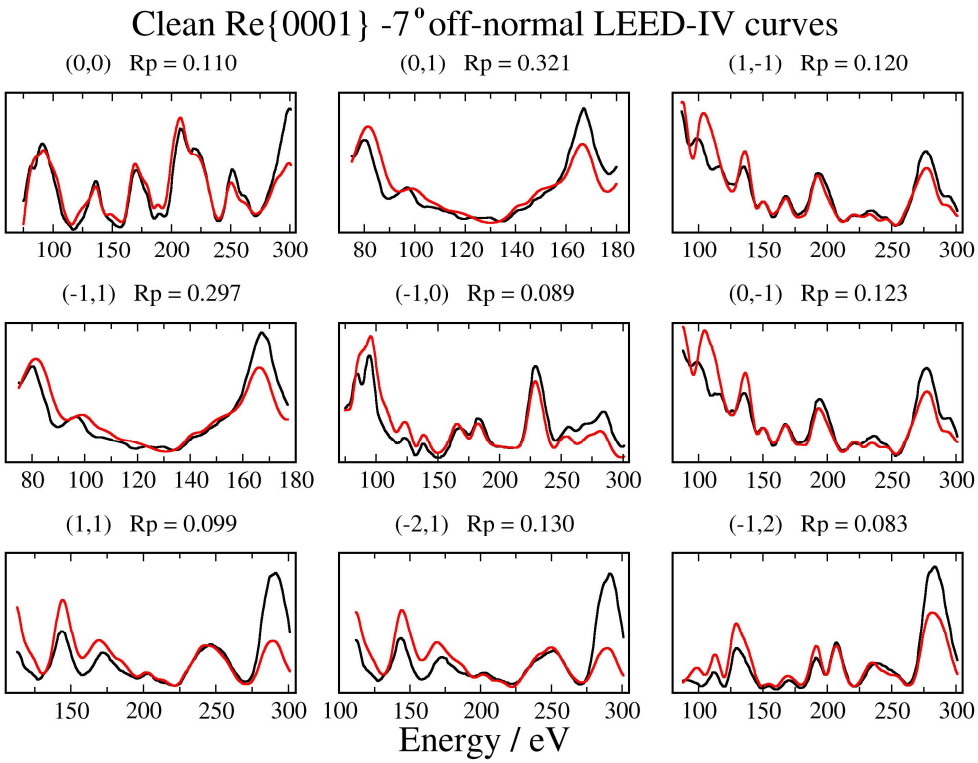
downhill simplex method was used for the structure optimization [2]. RR is the reliability of the R-factor (R_P), $RR = \sqrt{\frac{8V_i}{\Delta E}}$, where V_i is the optical potential and ΔE is the total energy range analysed.

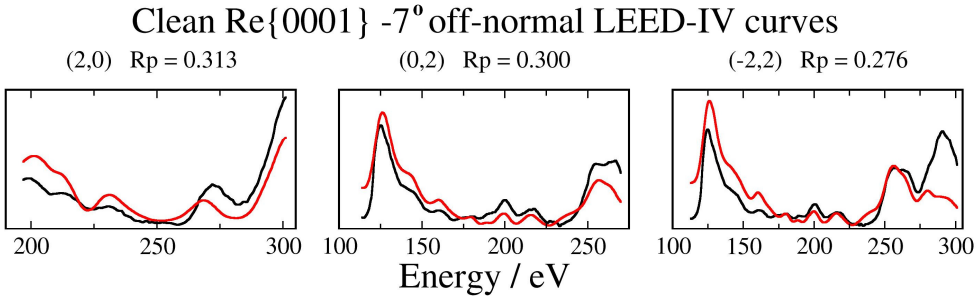
LEED-IV Figures

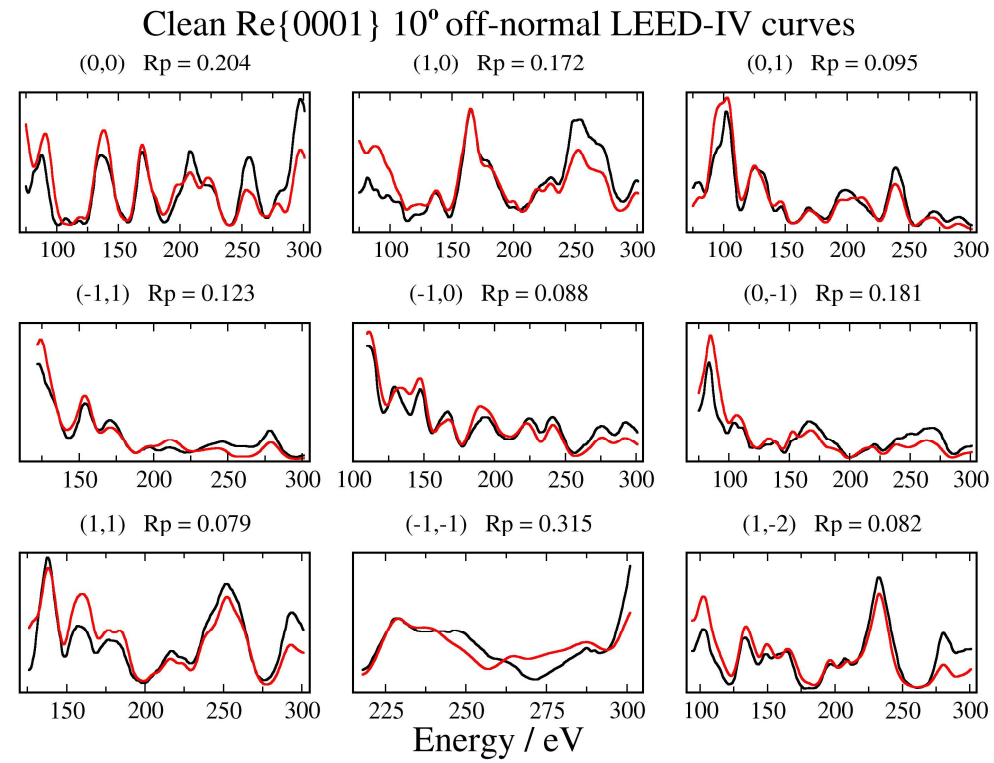
The full set of LEED-IV data and best fit curves are given in the following sets of images. For each the title is self explanatory and the black curves the data and the red curves the best fits. Individual R_P values are indicated for each fit.

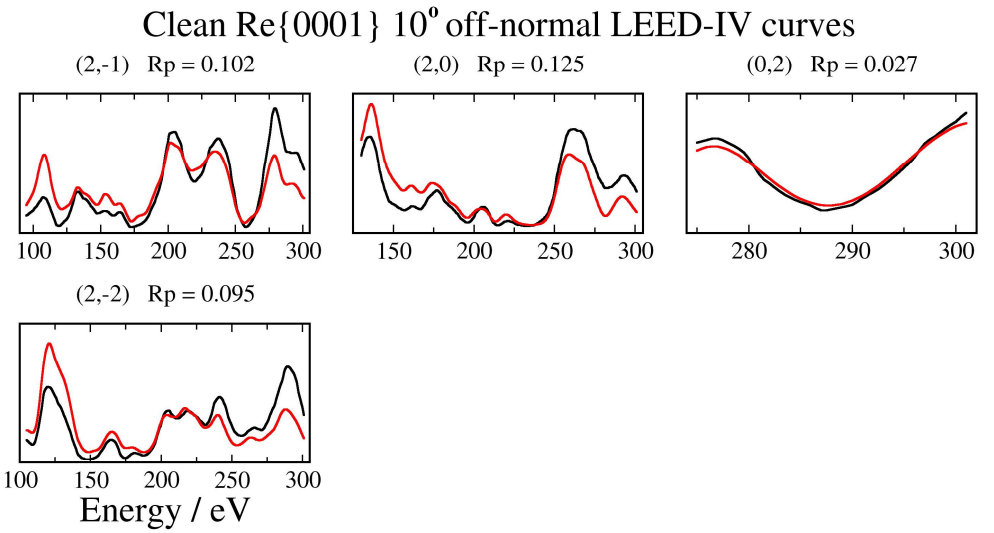



Clean Re{0001} 3° off-normal LEED-IV curves
(1,-2) Rp = 0.062
(-2,1) Rp = 0.050
(2,0) Rp = 0.141
(0,2) Rp = 0.096
(2,-2) Rp = 0.191
(-2,2) Rp = 0.143
(-2,0) Rp = 0.105
(0,-2) Rp = 0.139
175 200 225 250 275 300
150 200 250 300
150 200 250 300
150 200 250 300
175 200 225 250 275 300
175 200 225 250 275 300
240 260 280 300
240 260 280 300
Energy / eV

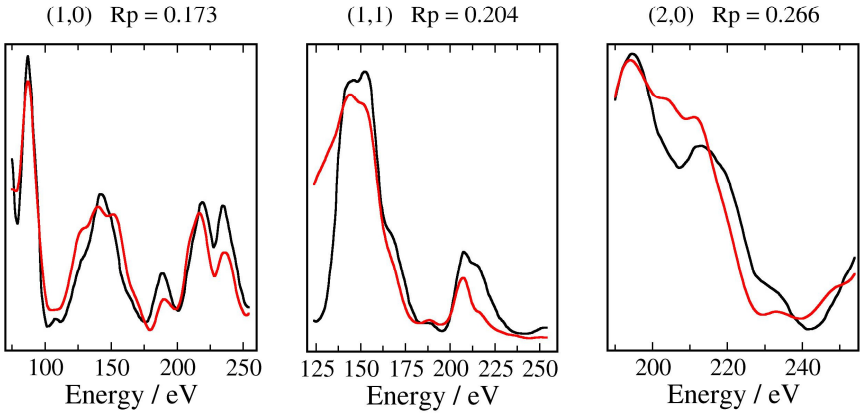

Clean Re{0001} -7° off-normal LEED-IV curves
(0,0) Rp = 0.110
(0,1) Rp = 0.321
(1,-1) Rp = 0.120
(-1,1) Rp = 0.297
(-1,0) Rp = 0.089
(0,-1) Rp = 0.123
(1,1) Rp = 0.099
(-2,1) Rp = 0.130
(-1,2) Rp = 0.083
Energy / eV


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

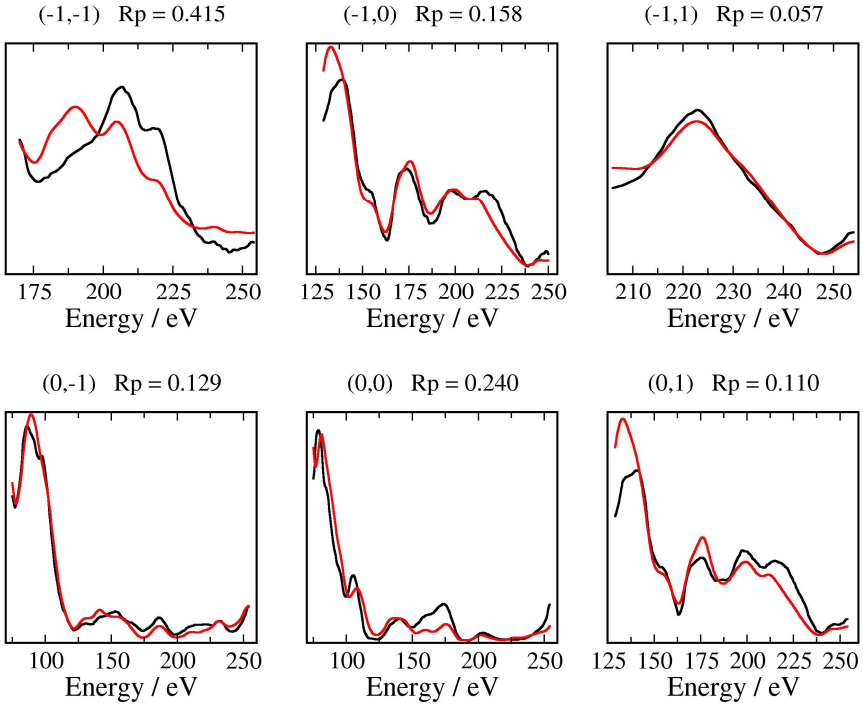

Clean Re{0001} 10° off-normal LEED-IV curves
(0,0) Rp = 0.204
(1,0) Rp = 0.172
(0,1) Rp = 0.095
(-1,1) Rp = 0.123
(-1,0) Rp = 0.088
(0,-1) Rp = 0.181
(1,1) Rp = 0.079
(-1,-1) Rp = 0.315
(1,-2) Rp = 0.082
Energy / eV

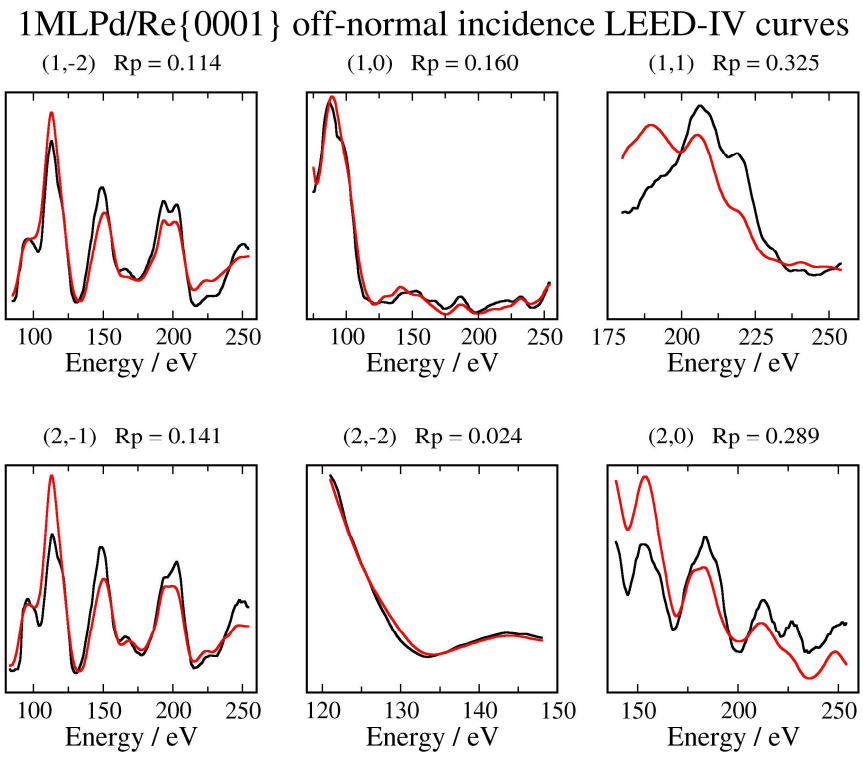

Clean Re{0001} 10° off-normal LEED-IV curves
(2,-1) Rp = 0.102
(2,0) Rp = 0.125
(0,2) Rp = 0.027
(2,-2) Rp = 0.095
Energy / eV

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

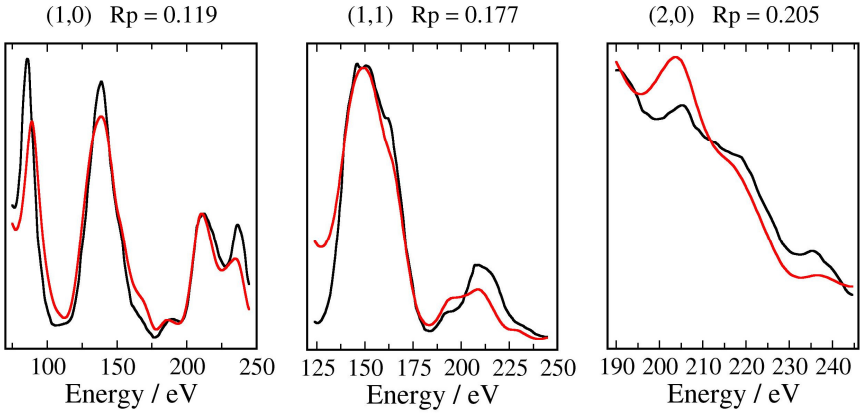


1MLPd/Re{0001} off-normal incidence LEED-IV curves

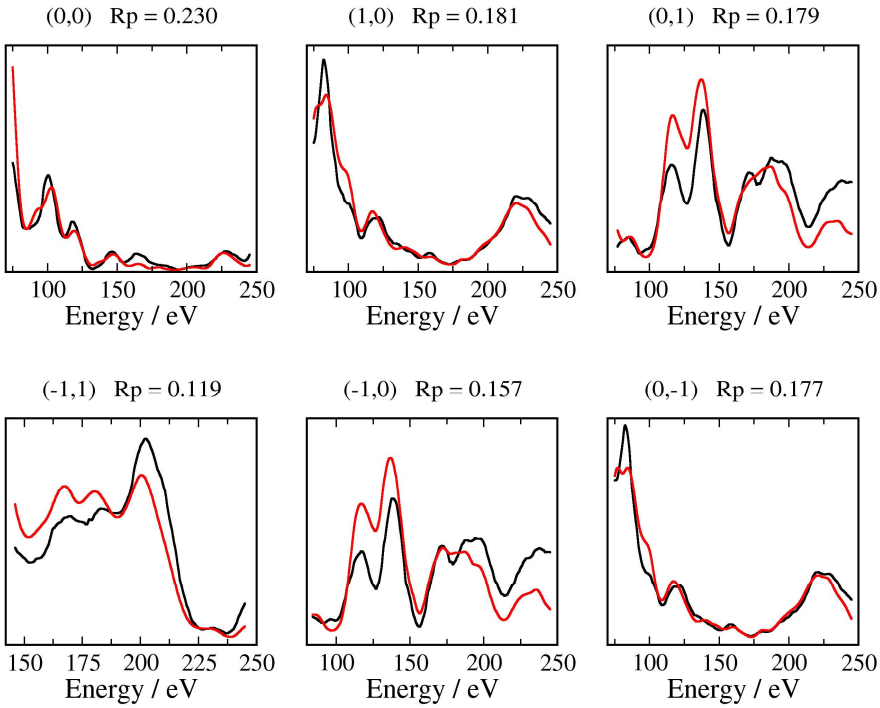


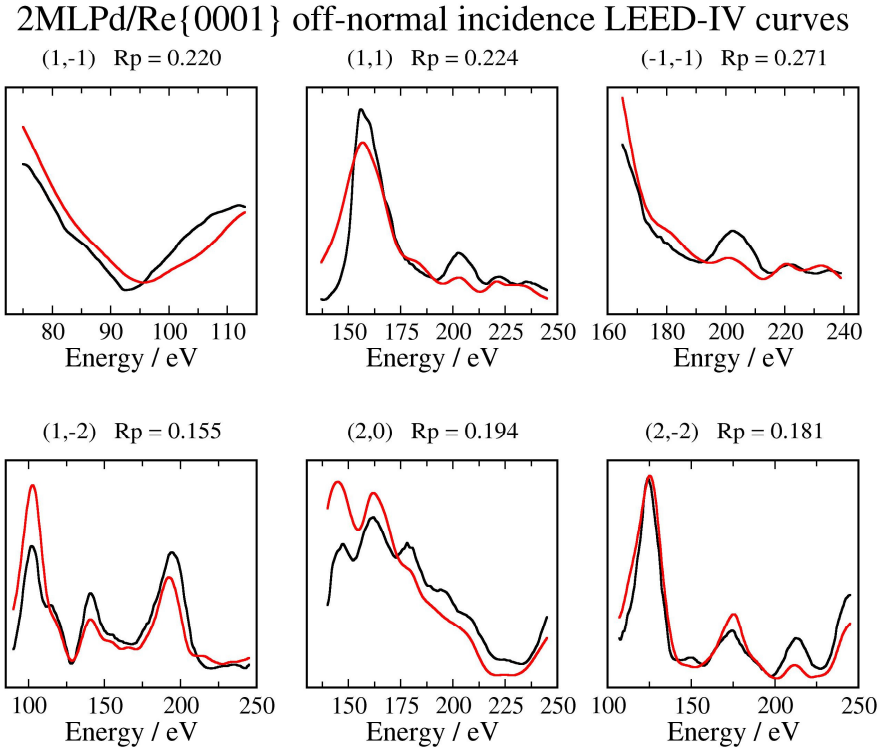

1MLPd/Re{0001} off-normal incidence LEED-IV curves
(1,-2) Rp = 0.114
(1,0) Rp = 0.160
(1,1) Rp = 0.325
(2,-1) Rp = 0.141
(2,-2) Rp = 0.024
(2,0) Rp = 0.289
100 150 200 250
175 200 225 250
120 130 140 150
150 200 250
Energy / eV

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

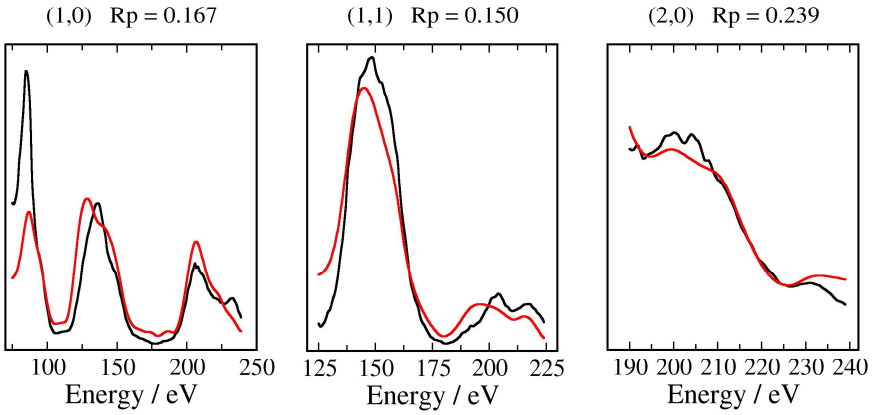


2MLPd/Re{0001} off-normal incidence LEED-IV curves

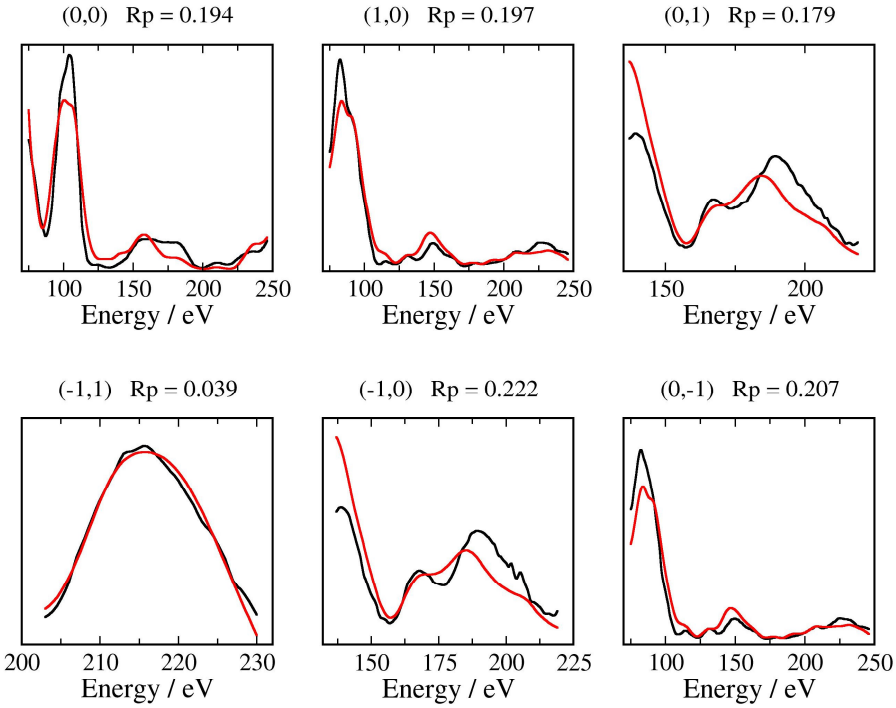


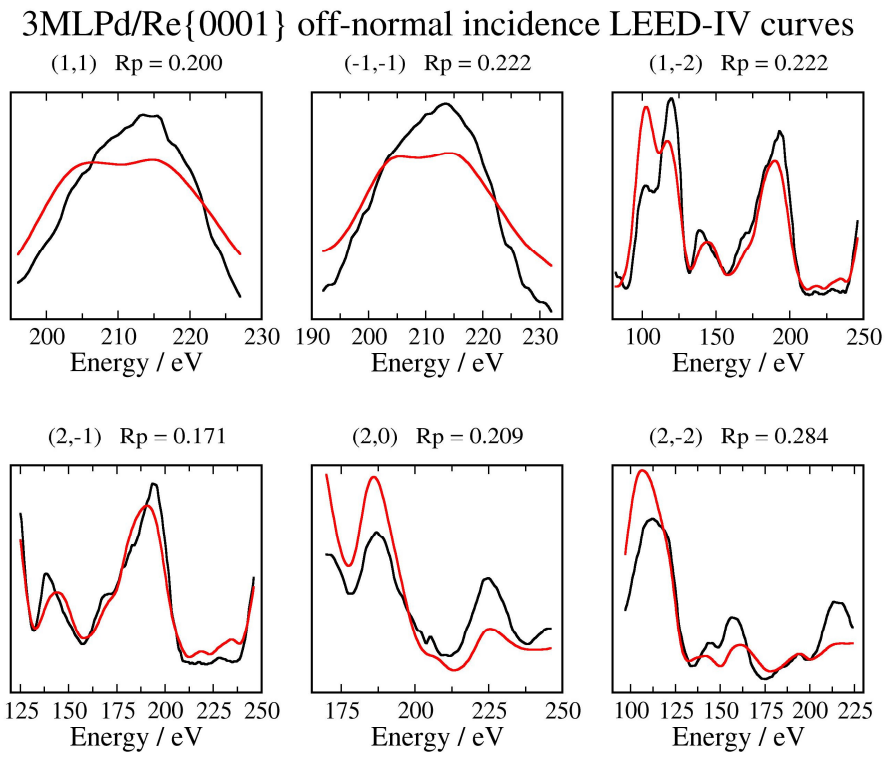

2MLPd/Re{0001} off-normal incidence LEED-IV curves
(1,-1) Rp = 0.220
80 90 100 110
Energy / eV
(1,1) Rp = 0.224
150 175 200 225 250
Energy / eV
(-1,-1) Rp = 0.271
160 180 200 220 240
Enrgy / eV
(1,-2) Rp = 0.155
100 150 200 250
Energy / eV
(2,0) Rp = 0.194
150 175 200 225 250
Energy / eV
(2,-2) Rp = 0.181
100 150 200 250
Energy / eV

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

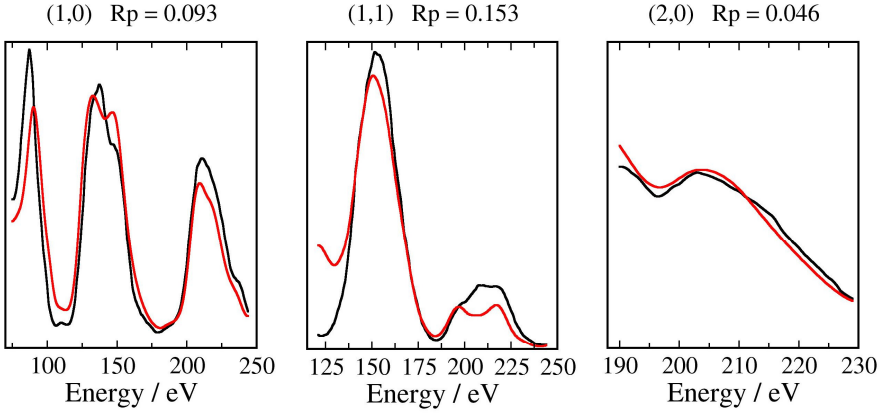


3MLPd/Re{0001} off-normal incidence LEED-IV curves

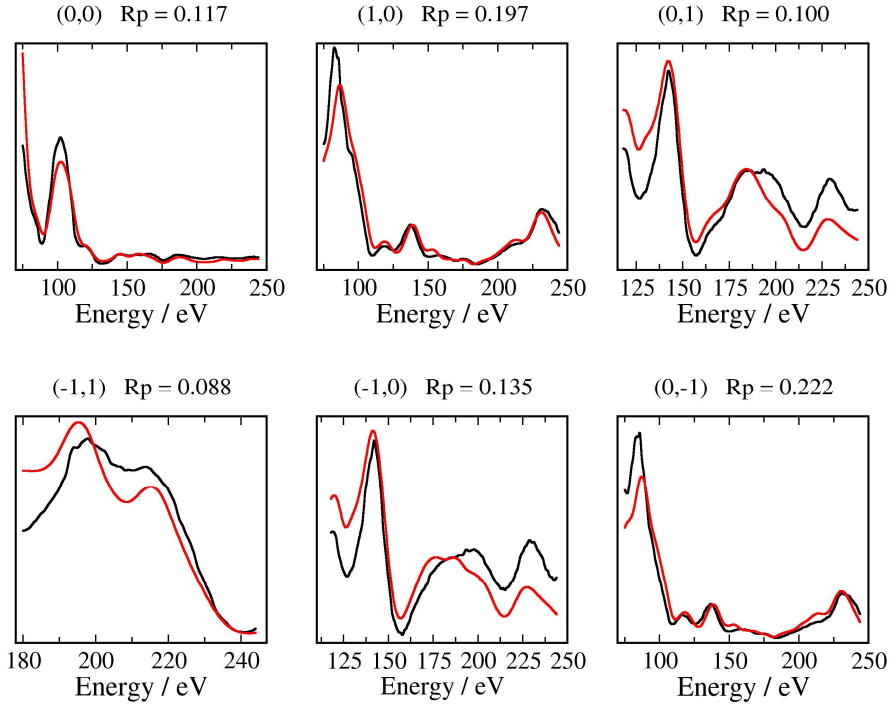


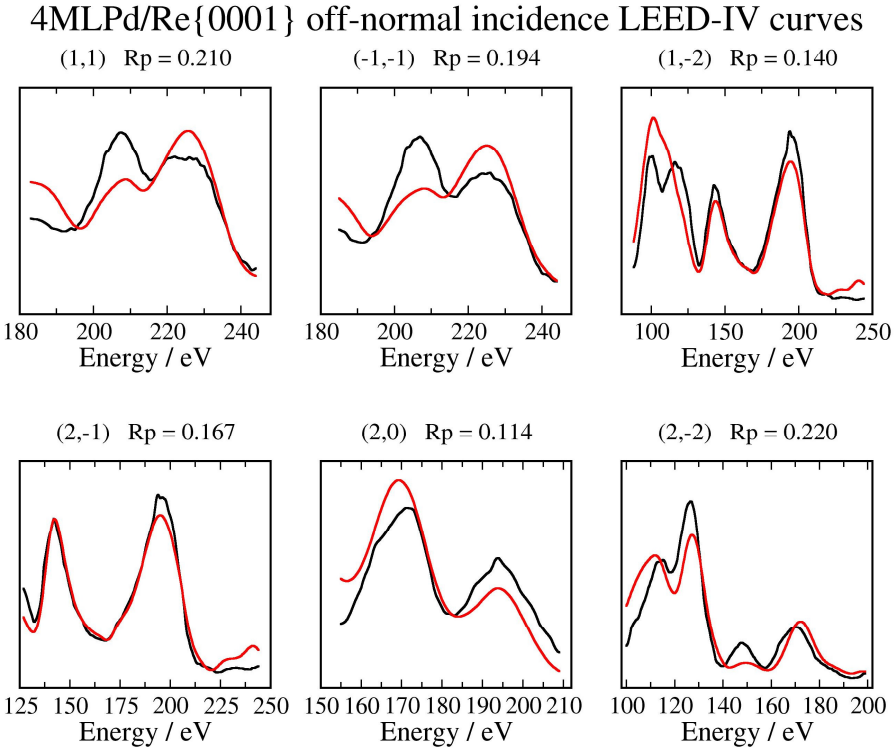

3MLPd/Re{0001} off-normal incidence LEED-IV curves
(1,1) Rp = 0.200
(-1,-1) Rp = 0.222
(1,-2) Rp = 0.222
(2,-1) Rp = 0.171
(2,0) Rp = 0.209
(2,-2) Rp = 0.284
Energy / eV

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



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





Supplementary References

1 Barbieri, A.; Van Hove, M. A. *Phase shift program package*, available from http://electron.lbl.gov/software/software.html

2 Press, W. H.; Flannery, B. P.; Teukolsky, S. A.; Vetterling, W. T. *Numerical Recipes in C*: Cambridge University Press: Cambridge, 1988.