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}

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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[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

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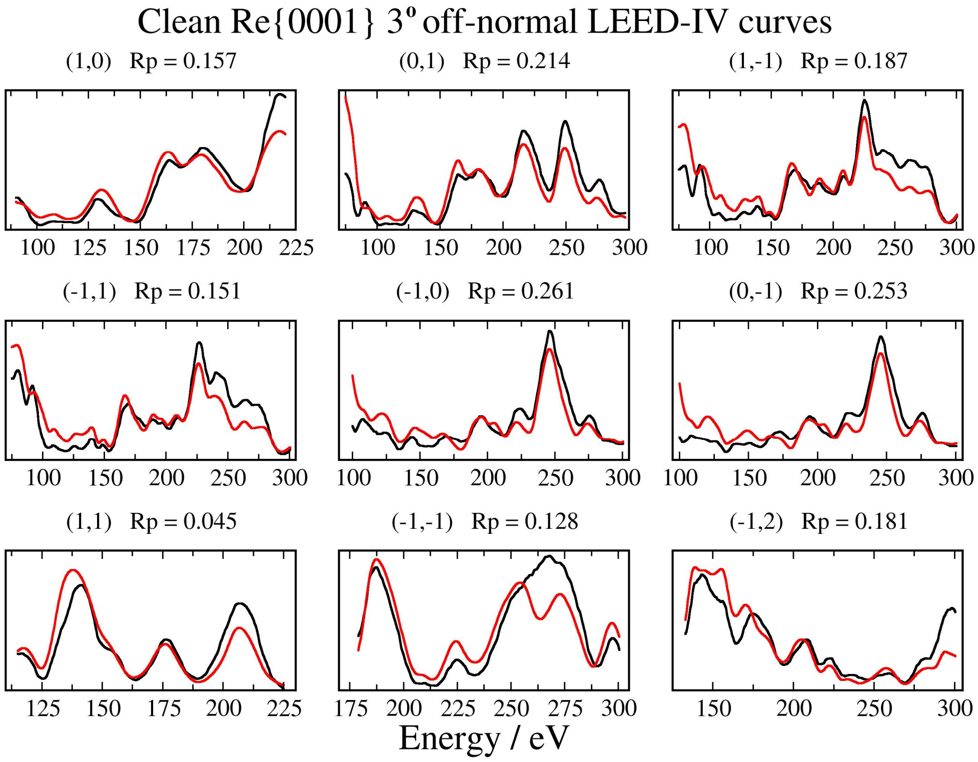
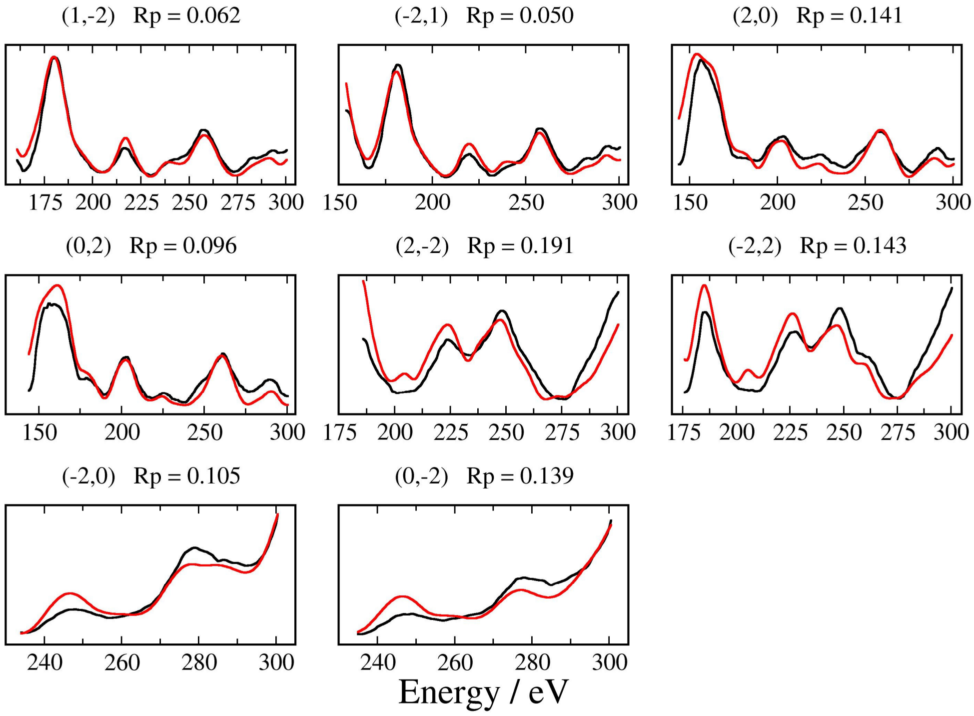
downhill simplex method was used for the structure optimization [2]. RR is the reliability of the R-factor (R_P), $RR = \sqrt{\frac{8V_i}{\Delta E}}$, where V_i is the optical potential and ΔE is the total energy range analysed.

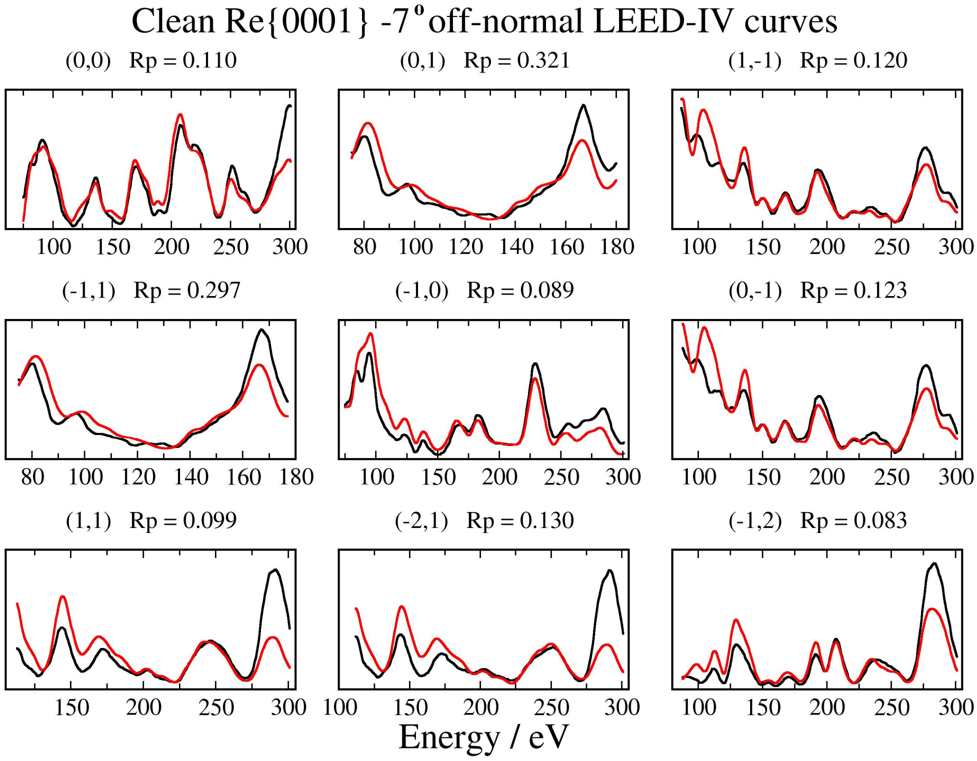
LEED-IV Figures

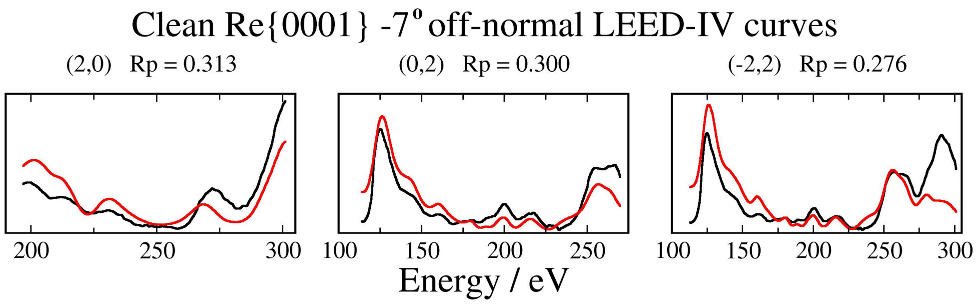
The full set of LEED-IV data and best fit curves are given in the following sets of images. For each the title is self explanatory and the black curves the data and the red curves the best fits. Individual R_P values are indicated for each fit.



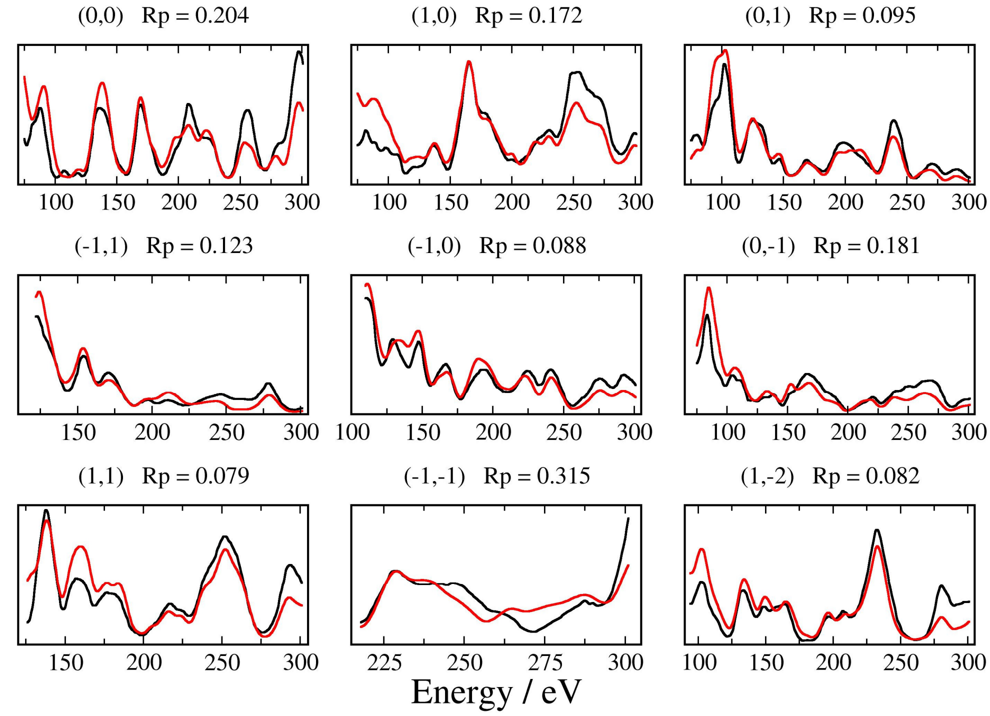
Clean Re{0001} 3° off-normal LEED-IV curves



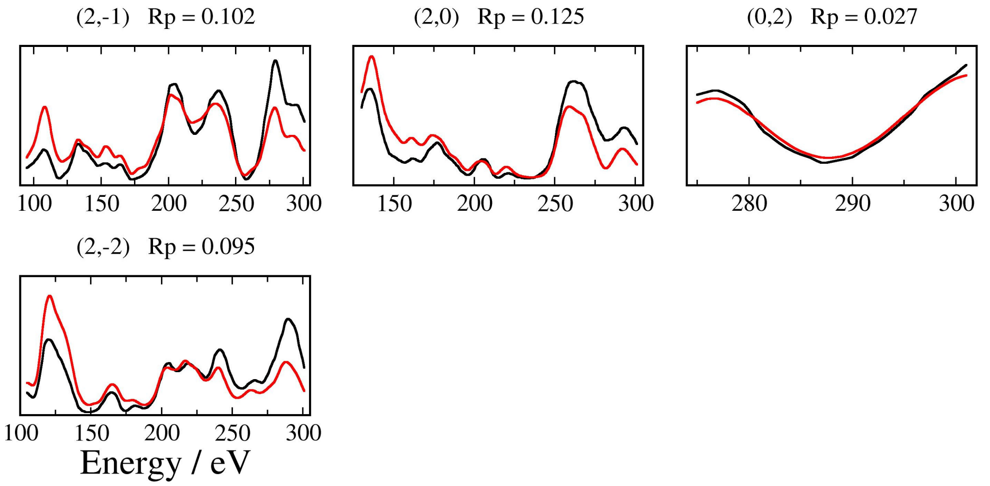

Clean Re{0001} -7° off-normal LEED-IV curves
(0,0) Rp = 0.110
(0,1) Rp = 0.321
(1,-1) Rp = 0.120
(-1,1) Rp = 0.297
(-1,0) Rp = 0.089
(0,-1) Rp = 0.123
(1,1) Rp = 0.099
(-2,1) Rp = 0.130
(-1,2) Rp = 0.083
Energy / eV


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

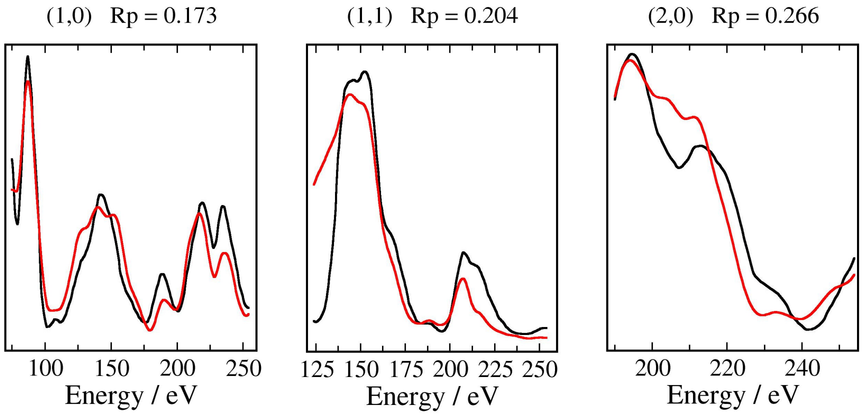
Clean Re{0001} 10° off-normal LEED-IV curves



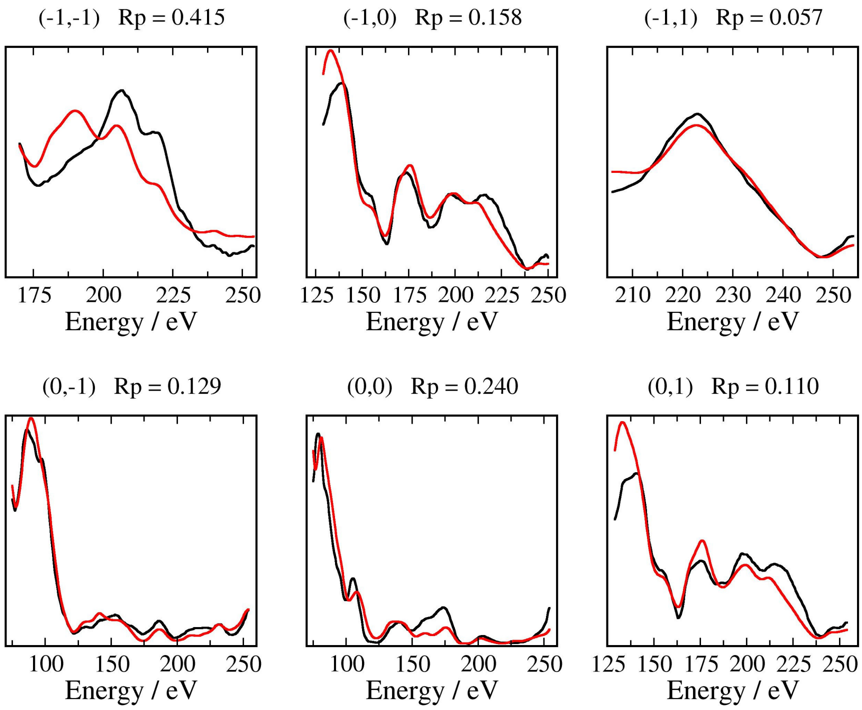
Clean Re{0001} 10° off-normal LEED-IV curves



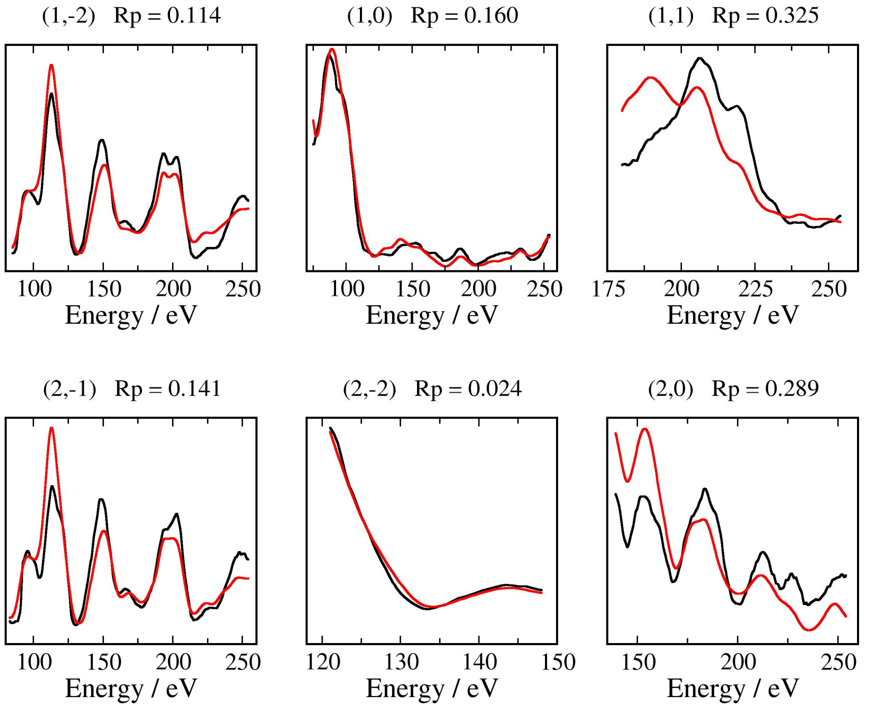
1MLPd/Re{0001} normal incidence LEED-IV curves



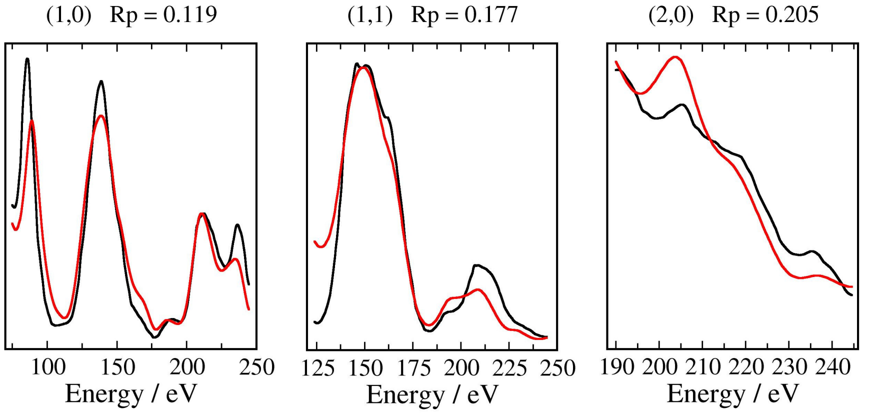
1MLPd/Re{0001} off-normal incidence LEED-IV curves



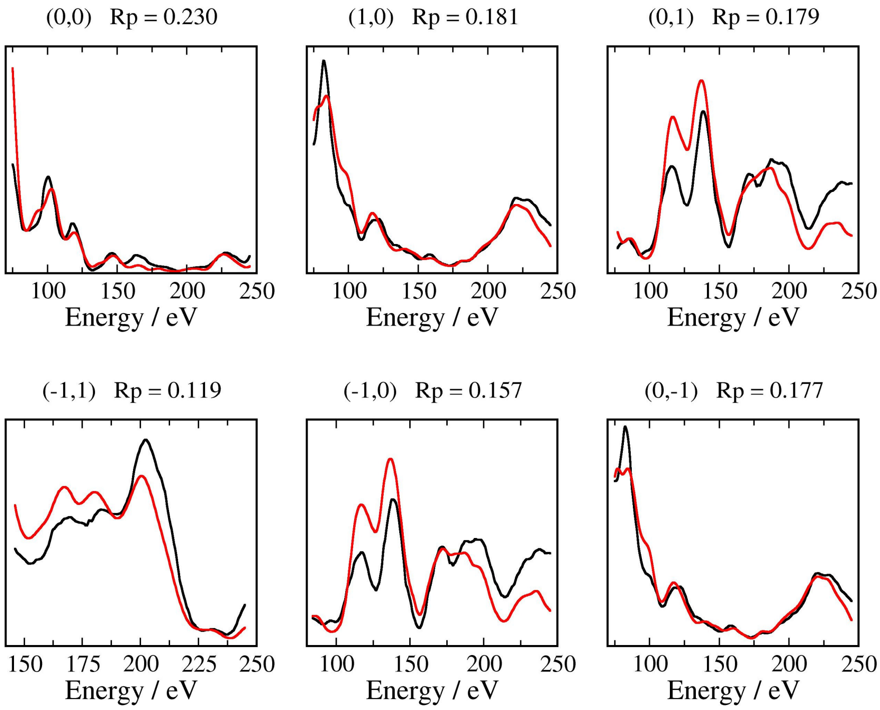
1MLPd/Re{0001} off-normal incidence LEED-IV curves



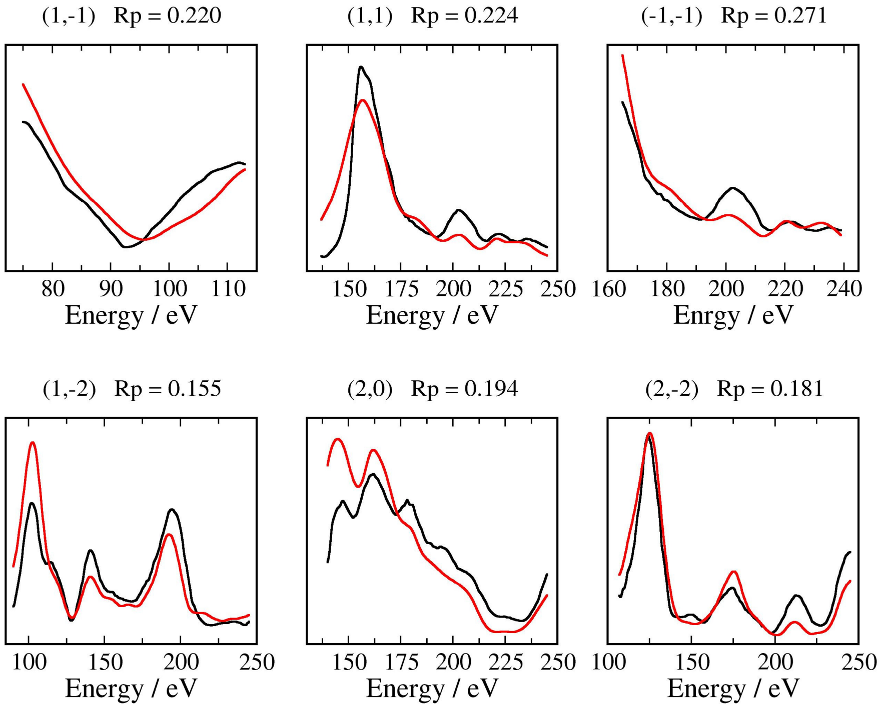
2MLPd/Re{0001} normal incidence LEED-IV curves



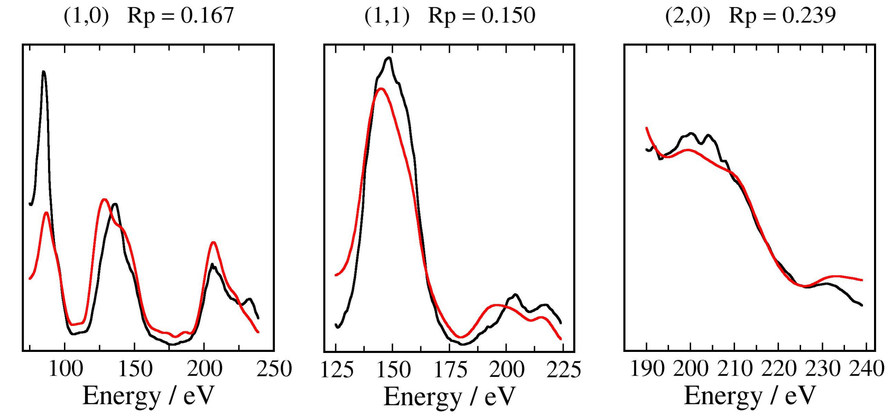
2MLPd/Re{0001} off-normal incidence LEED-IV curves



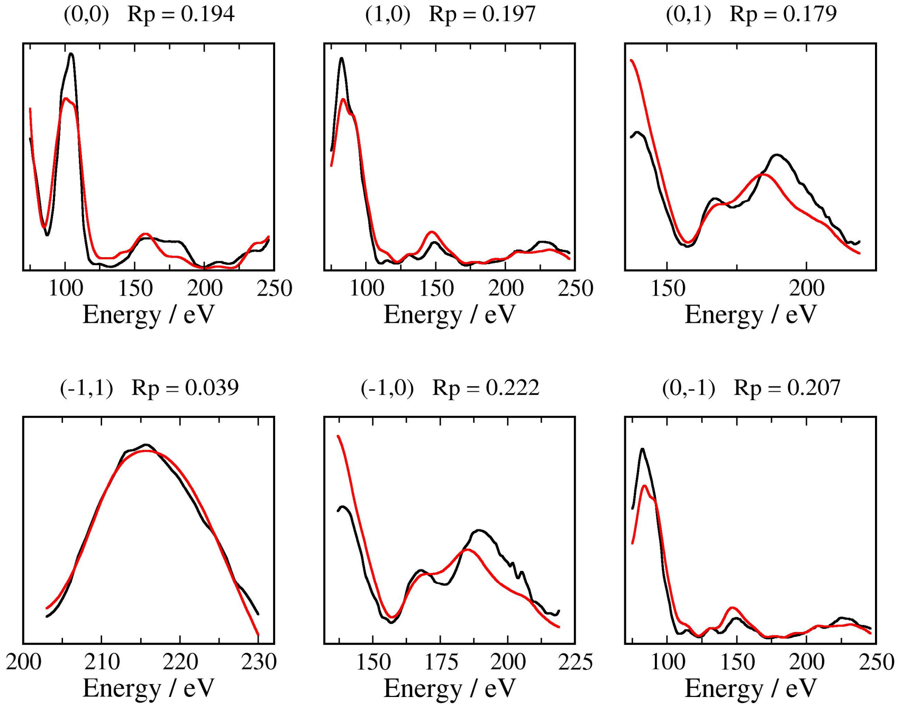
2MLPd/Re{0001} off-normal incidence LEED-IV curves



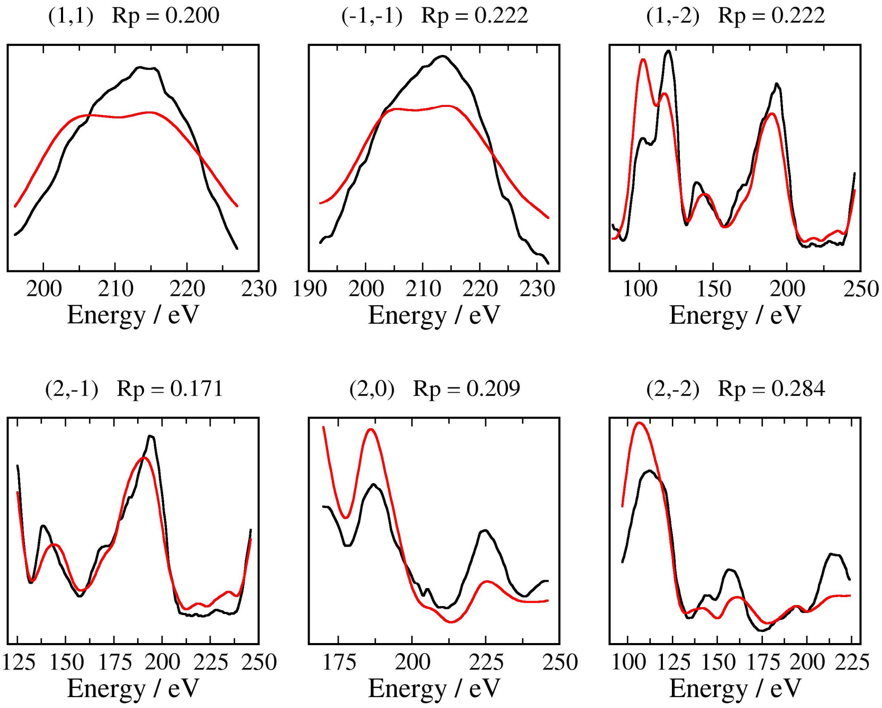
3MLPd/Re{0001} normal incidence LEED-IV curves



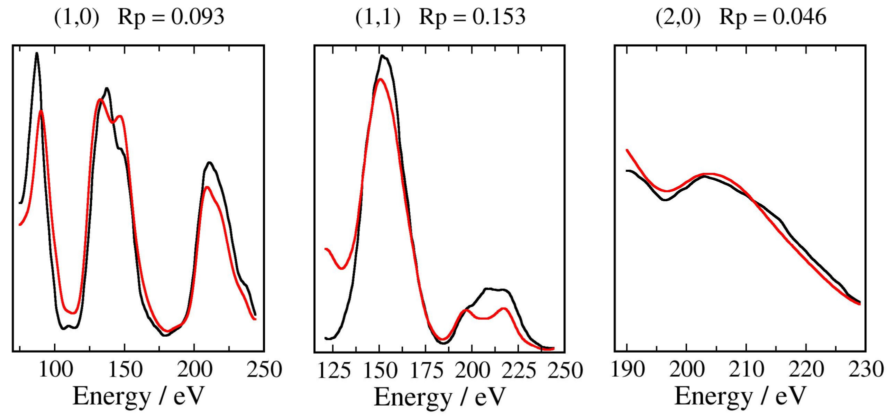
3MLPd/Re{0001} off-normal incidence LEED-IV curves



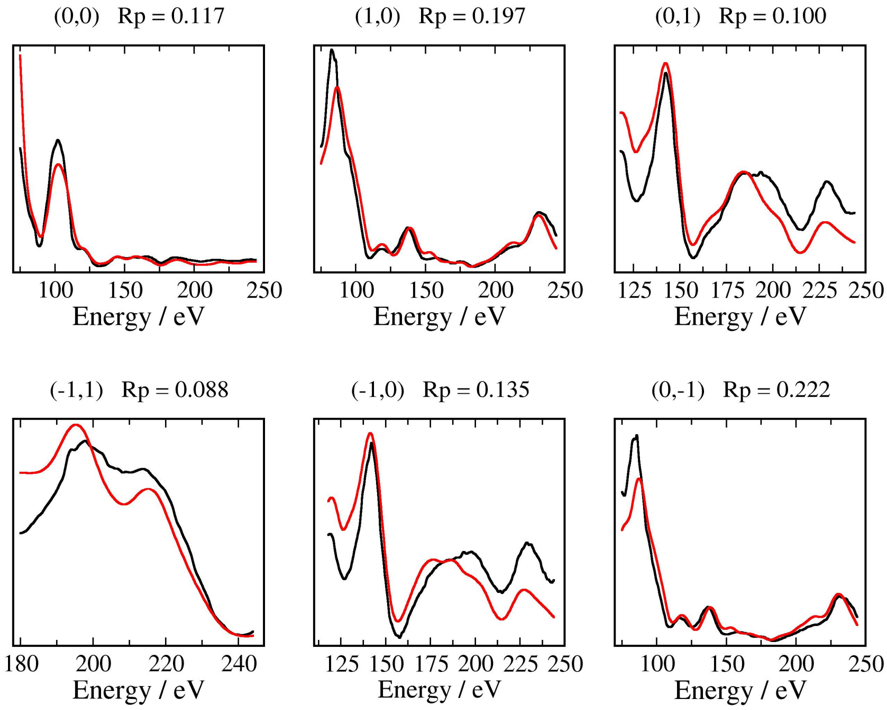
3MLPd/Re{0001} off-normal incidence LEED-IV curves



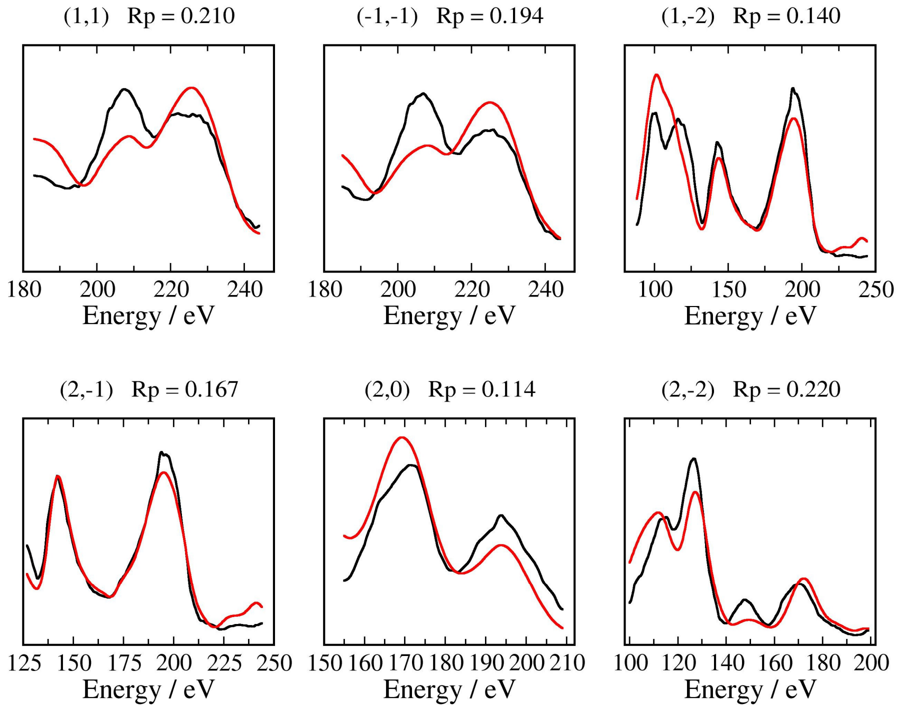
4MLPd/Re{0001} normal incidence LEED-IV curves



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



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



Supplementary References

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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.