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Surface Relaxation of V(100); Experiments and Ab-Initio Calculations: a status report on the Feibelman Issue D. LACINA, A. CIUCIVARA, B.R. SAHU, L. KLEINMAN, J.L. ERSKINE, Physics Dept., Univ. of Texas, Austin — Systematic discrepancies between first-principles calculations and experimental determinations of the surface relaxation of reactive transition metals was first noted by Feibelman.[1] The basic issue is that calculations invariably yield first- layer (inward) relaxations that substantially exceed the results obtained by electron diffraction, and the disagreement lies beyond the accepted accuracy of the experiments and calculations. We report new LEED results and calculations for V (100) that explore this trend and present a status report on the primary issues. The LEED results for several data sets at 300 K and 100 K are robust and consistent with d_{12} = -5.0 $\pm$1.0 % and d_{23} = 3.6 $\pm$1.0 %with acceptable Pendry and Zanazzi-Jona r-ractors. Preliminary calculations using pseudopotentials without partial core corrections gave d_{12} = -14.0 % in the GGA (cf. the more accurate FPLAPW d_{12} = -11.1 %).[2] Meta-GGA[3] calculations resulted in d_{12} = -12.0 % suggesting meta-GGA FPLAPW calculations might yield d_{12} as small as -9 %, still an unacceptably large deviation from experiment.
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