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The effect of select non-structural parameters upon the intensity of calculated LEED I(E) curves NATHAN GRIESER, Ohio Northern University — The LEED investigation of the (5x5) structure formed by sulfur adsorbed on a clean Au(111) surface results in calculated I(E) curves which exhibit unexpectedly low intensity at high energies of the probing electrons. The present study investigates various parameters used in the dynamical LEED calculation these curves, which are predominantly responsible for the intensity of the curves. Parameters such as: the Debye temperature associated with the sulfur adsorbed layer, the imaginary part of the inner potential describing the inelastic energy losses of the probing electrons within the crystal, and the anisotropic vibrations of the sulfur layer (enhanced vibrations in a direction perpendicular to the surface) have been studied by monitoring their effect on the intensity of the calculated curves. Also, the phase shifts describing the scattering of the incoming electrons by the S and Au atoms have been calculated for different configurations of the sulfur atoms on the substrate, and their influence on the I(E) curves has been considered. It is concluded that even if a certain enhancement of the beams' features is possible by choosing a particular combination of the above mentioned parameters, the process of comparing the experimental and theoretical beams by mainly matching the peak positions (as done by the Pendry R factor) imposes certain values of these parameters, not necessarily the ones which would produce high intensity peaks.

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