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Low-Energy Electron Diffraction Investigation of the Cu(511) Stepped Surface CHRISTOPHER LEMON, MELLITA CARAGIU, Ohio Northern University, RENEE DIEHL, KELLY HANNA, HSIN LI, RUNDONG WAN, Pennsylvania State University — Preliminary results concerning the investigation of the clean Cu(511) (stepped) surface are presented with emphasis on the computation part of the investigation. Low-energy electron diffraction (LEED) calculations applied to stepped surfaces are usually associated with convergence problems due to the very small interlayer spacing of the sample to be investigated [K. Pussi, M. Caragiu, M. Lindroos, R.D. Diehl, Surf. Sci. 544 (2003), 35]. Therefore, composite layers made of several (7-10) close-spaced layers have been used in resolving the clean Cu(511) structure employing the TLEED (Tensor LEED) computer software [A. Barbieri, P.J. Rous, A. Wander, M.A. Van Hove, Automated Tensor LEED Programs]. Ideally, the electron beam diffracted by the sample should hit the surface under normal incidence. This is, however, hard to control due to the existence of only one symmetry plane of the real structure, which, in turn, gets translated into only one symmetry plane in the reciprocal space. The uncertainty in the angle of incidence makes the angle itself a variable parameter in the LEED calculation, beside the usual parameters to be fitted during the calculation.

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