

Abstract Submitted
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Global optimization in surface structure determination by electron diffraction using generalized pattern search methods¹ ZHENGJI ZHAO, JUAN MEZA, CRD, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, MICHEL VAN HOVE, MSD and ALS, Lawrence Berkeley National Laboratory, Berkeley, CA 94720; Dept. of Physics, University of California, Davis, Davis, CA 95616 — Low energy electron diffraction (LEED) is the most commonly used method for detailed surface structure determination. This method can be formulated as an inverse problem, by attempting to fit dynamically calculated LEED intensities to experimental data. As with any such method, it faces a challenging global optimization. We discuss the use of generalized pattern search (GPS) methods for this global optimization, using the complex Ni(001)-(5x5)-Li structure as an example. We present numerical results for one particular GPS method (NOMAD) and compare its performance to previously used genetic algorithm methods.

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