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APPLICATION OF GENETIC ALGORITHMS TO SURFACE X-RAY DIFFRACTION ANALYSIS

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A precise knowledge of the crystalline structure of a surface is one of the most important aspects required to understand its properties [1]. SXRD is one of the most powerful techniques sensitive to long-range order. A generalized use of SXRD as a standard technique has been hindered by several difficulties, one of them being the fact that if the surface structure is complex, with several different adsorption sites and a large unit cell, the process of fitting an SXRD dataset can be long and tedious. In this contribution we introduce the use of genetic algorithms [2] for the analysis of SXRD data, taking into account its specificities, and compare their features with other methods commonly used, like simulated annealing or Levenberg–Marquardt algorithms. We also present the analysis of the surface structure of Sn/Cu(100)-(3√2×√2)R45◦ using these methods. This structure has been analyzed in detail using dynamic LEED, so that the results of the use of a genetic algorithm can be compared easily to previous structural data. We find a good agreement between dynamic LEED results, and sometimes an almost exact coincidence, with most of the distances obtained in this work from SXRD and using the differential evolution algorithm for the optimization of the fit.

As there are no precedents in the use of this algorithm for the crystallographic analysis using SXRD, these findings support the validity of the method, which is found to be a promising and powerful tool in the analysis of this kind of problem [4]. It is able to extract crystallographic information in a fast and reliable way, in spite of the large size of the unit cell and the significant number of parameters fitted. A general comparison with other methods is difficult, as only the Levenberg–Marquardt and the *simulated annealing* method are actually implemented in a fitting code of widespread use. While these methods are useful for the refinement of a model, the genetic algorithm appears as a much powerful and fast method to discriminate between possible models and to find the best structure for a certain model, *i.e.* in what concerns the uniqueness and reliability of the model found, mainly due to the much broader range of structures probed in a systematic way.

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