Genetic Algorithm For Crystal Structure Prediction

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The development of methods for solving the problem of crystal structure prediction has also been motivated by a growing range of applications where reliable structure prediction is sought and could guide experimentation. The prediction of crystal structures are extremely interesting because of their applications are completely related to the crystal structure. A total 3N+3 dimensions describes the atomic coordinates and lattice vectors of a crystal structure, itself must be determined the crystal structure prediction and the data is collected by X-ray diffraction. There are several methods are used to predict the crystal structure.In this a genetic algorithm has been used to generate plausible crystal structure from the knowledge of only the unit cell dimensions and constitute elements. This research is attempted to predict the crystal structure using genetic algorithm by using X-ray diffraction data.

Potassium Di-hydrogen Phosphate (KH_2PO_4) single crystals have high laser damage threshold, large nonlinear optical coefficients, good structural quality and mechanical properties. KDP crystals have several device applications. The electro-optic effect in KDP is used to obtain phase and amplitude modulations. The rapid growth technique supplied us with the big crystals of low cost and equivalent optical quality as well as rapid growth of KDP crystals with additives have facilitated to obtain perfect KDP crystals for device application on large scale. Huge interest to KDP crystals is caused by their unique physical properties and high manufacturability. In particular, KDP crystals which possess extremely high optical and structural perfection make it possible to produce elements for doubling 165 and tripling of laser radiation frequency, electro-optic switches and modulators with an aperture of several tens and hundreds of square centimeters to be used**.** X-ray diffraction patterns were studied for material identification and structural analysis.

Genetic Algorithm is started with a set of solutions (represented by individuals) called population.Solutions from one population are taken and used to form a new population. This is motivated by a hope, that the new population will be better than the old one. Solutions which are selected to form new solutions (offspring) are selected according to their fitness - the more suitable they are the more chances they have to reproduce. This is repeated until some condition (for example number of populations or improvement of the best solution) is satisfied(figure).

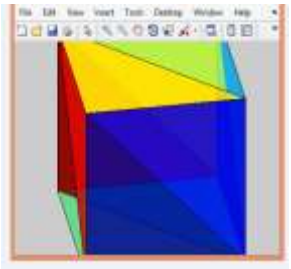

figure 1 (screen shot of best individual after the iteration)