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Inverse design of materials by multi-objective differential evolution

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ABSTRACT

Inverse design is a promising approach in the realm of material science for finding structures with desired property. We developed a new package with novel algorithm for inverse design named as IM^{2}ODE (inverse design of Materials by Multi-Objective Differential Evolution). The target properties of concern include the optical and electronic-structure properties of semiconductors, hardness of crystals, etc. IM^{2}ODE can easily predict the atomic configurations with desired properties for three dimensional structure, interface and cluster, even complex defect in solid. Tests have been run on multiple systems and it has been proved that IM^{2}ODE is highly efficient and reliable, which can be applied widely.

1. Introduction

Traditionally discovering new materials is a long and costly process including a huge amount of trial and error in the progress of synthesizing and testing. Theoretical designing of materials has been a long standing dream of the scientists. With the development of supercomputers and first principle methods, one can correctly predict most of the properties of a material if the atomic configuration is known. However, the inverse of this approach, finding a material with unknown structure and desired properties, is still a great challenge in material design.

One way to do inverse design is by scanning databases of structures previously found and substituting elements in those structures, which is known as 'high-throughput' (HT) computational materials design, focusing on finding different composites of compounds [1–7]. Another way is to figure out the atomic configuration of a fixed chemical system with the desired properties, which is often achieved by combining an atomic structure searching with first principle calculations of target properties. These methods were first proposed by Franceschetti and Zunger, using simulated annealing algorithm to predict the atomic configuration of $Al_{0.25}Ga_{0.75}As$ alloy with the largest optical band gap [8]. Later, genetic algorithm [9,10] and particle swarm optimization [11,12] are proposed to design ordered alloy and meta stable crystal phase with target electronic-structure property. However, these methods take desired properties into account while neglecting the total energy and it is possible that the structures found by those methods may have rather high energy.

Atomic structure is the most fundamental properties of materials. In the past two decades, quite a few global optimization methods were developed to search the atomic structures [13–17]. Some global optimization packages, such as USPEX [18] and CALYPSO [19], were developed to predict new crystal structures with lowest enthalpy at given external conditions (e.g., pressure). The process of structure prediction involves exploring the energy surface which involves a huge number of energy minima. Highly efficient and robust global optimization methods are applied to solve this problem for sampling the energy surface and find global minima. There is something in common between the structure prediction and inverse design: both of them needs to scan the energy surface. The key difference is that structure prediction only needs to find a structure with the lowest energy, while inverse design needs to find a structure with desired properties.

Based on global optimization methods, we have developed a novel method for "inverse design", which is named as IM^{2}ODE (inverse design of Materials by Multi-Objective Differential Evolution). In this code package, Multi-Objective optimization methods are applied to predict structures with respect to both total energy and properties. By extending the inverse design problem from the single-objective domain to the multi-objective domain, we are able to predict metastable structures of desired properties with relatively low energy. Among the numerous global optimization algorithms, Multi-Objective Differential Evolution (MODE) has been widely used and achieved great successes [20–22]. MODE is

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based on Differential Evolution (DE), which is an evolutionary algorithm that optimizes an objection function by maintaining a population of candidates and creating new ones through mutation and crossover operations based on the differentials of the existing ones [23,24]. Greedy strategy is taken by the algorithm only keeping new candidates which out-perform the old ones. The evolutionary nature of the DE algorithm makes it a very effective solver for complex search problems, including either global or multi-objective problems, have already been applied for structure searching of cluster and interface [25,26]. Therefore MODE algorithm is suitable to be applied to the inverse material design problem.

This rest of the paper is organized as follows. In Section 2, the detailed description of IM^{2}ODE code is presented. In Section 3, some applications and tests of the method are given, followed by the conclusion in Section 4.

2. Algorithm

Different from the well-known structure search which is essentially single objection optimization, the nature of inverse material design is a multi-objective optimization. For instance, if we want to find suitable material for solar absorber, at least both band gap and total energy should be set as criteria. Therefore a multi-objective optimization method is necessary and here we adopt MODE algorithm. Generally, IM^{2}ODE package can be also applied to single objective problem, such as finding the most stable structure of complex systems of clusters on surfaces and interface of crystals. There are mainly four steps in the IM^{2}ODE code package: (i) generation of atomic structures, such as two-dimensional material, cluster, surface, interface or defect; (ii) local optimization of structures; (iii) sorting the structures in the solution space and finding duplicate structures; (iv) generation of new structure by DE or MODE operations. The main procedure of IM^{2}ODE package is shown in Fig. 1.

2.1. Generation of structure

Here we perform inverse design of materials including crystal, two-dimensional material, cluster, surface, interface and defect [16,18,27–30]. In the multi-dimensional search problem, an individual crystal structure is defined as a vector of dimension 3N + 6, which contains six lattice parameters, including three angles and three vectors, and 3N atomic coordinates of N atoms. The crystal structures are initialized considering the symmetry of the 230 space groups. The definition of two-dimensional materials is similar to that of crystal, and the only difference is that constrain is applied on the third dimension. There are three modes to initialize cluster, which are ball, shell and plate. To design the adsorption of cluster on solid surface, we place a surface below randomly generated cluster to obtain the best configuration of cluster, which dimension is the same as cluster. The interface is simulated with a slab model, containing fixed layer, rigid layer and optimized layer. The rigid layer can move as a whole and the atoms inside the interface are allowed to move for optimization. The dimension of the vector of interface is 3N + 3, which contains the atomic coordinates of the N atoms and the movement of the rigid layer [25].

2.2. Structural optimization

In principle, one can use any method for the structure optimization. Presently, we adopt Ab initio package VASP (*Vienna* ab initio *simulation package*) [31] to perform structure optimization and electronic structure calculation, of course we have successfully use classical potentials to perform the structural optimization of large system such as the structural search of grain boundary in graphene. In order to increase the efficiency, atomic coordinates and lattice parameters of the structures are locally optimized after initialization which can reduce the noise in the complex searching space and simplify the task of finding the global minimum on the

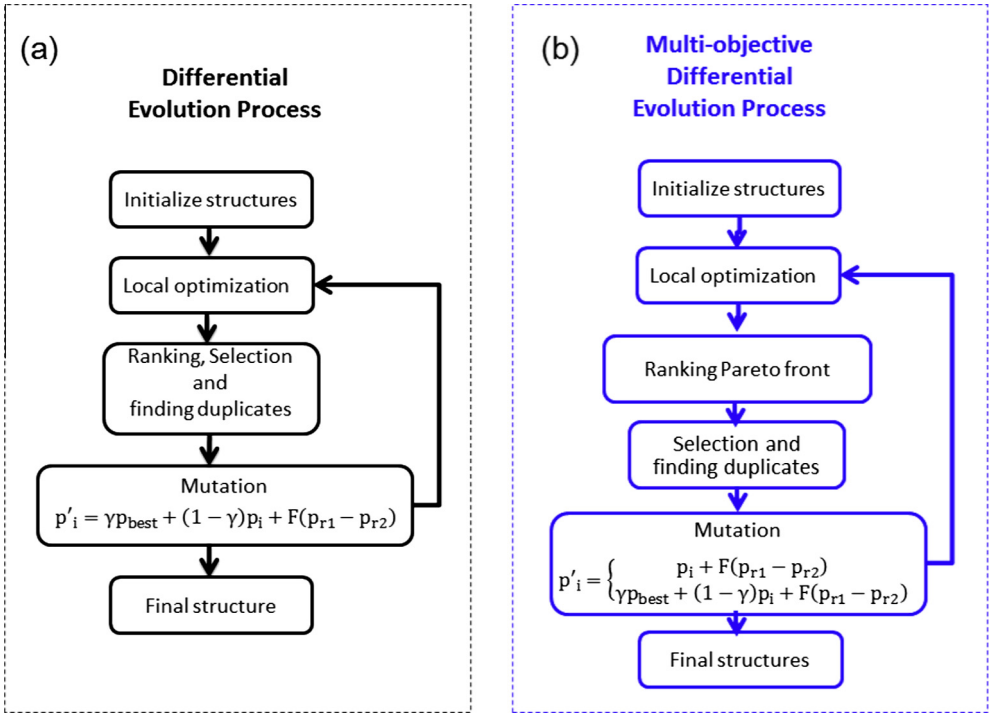

Fig. 1. Procedure of the IM^{2}ODE package including both DE process for single objective optimization (a) and MODE for multi-objective optimization (b). In the initialization step, crystal, two-dimensional material, cluster, surface, interface and defect can be generated. After that, local optimization of structures, ranking, selection, and mutation are performed iteratively until a predefined generation is reached and finally find out the optimized structure.